Materials from Topological Quantum Chemistry

Maia G. Vergniory

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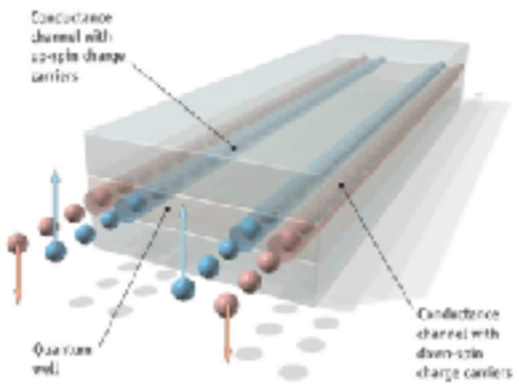
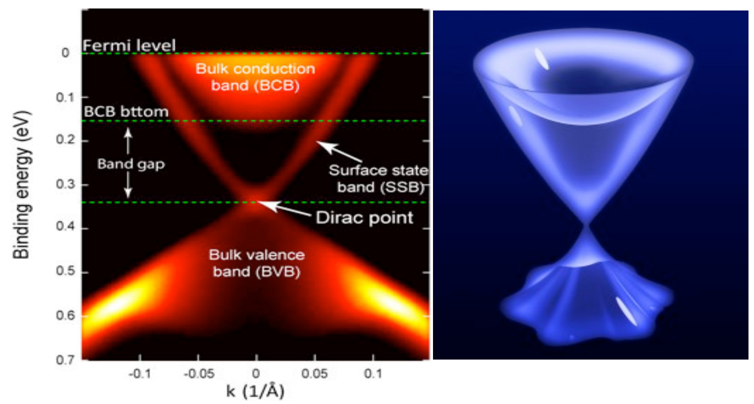
1709.01935, arXiv:1709.01937

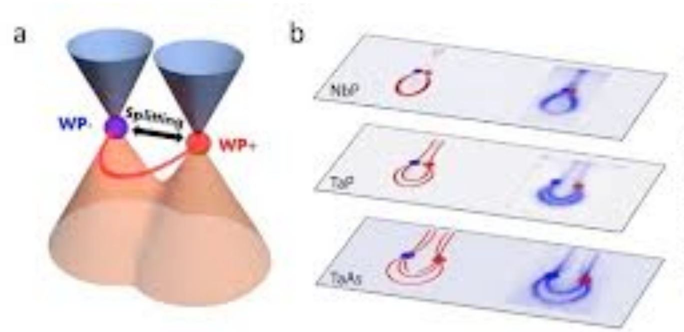
Topological Insulators and Topological Semimetals

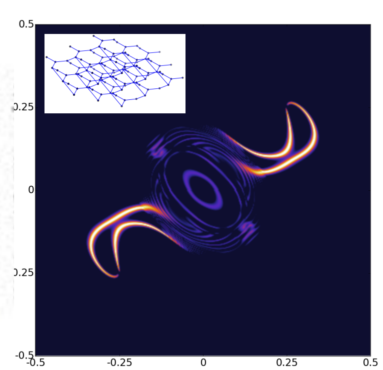




Topological Insulators /
Dirac Fermions

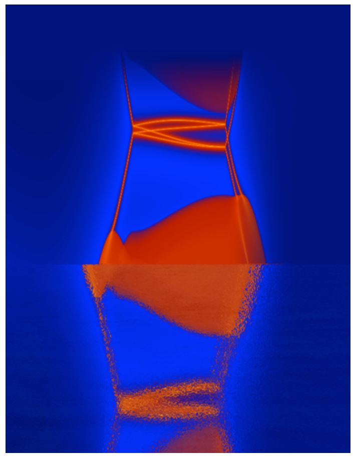
Topological protection from time reversal or some crystal symmetry

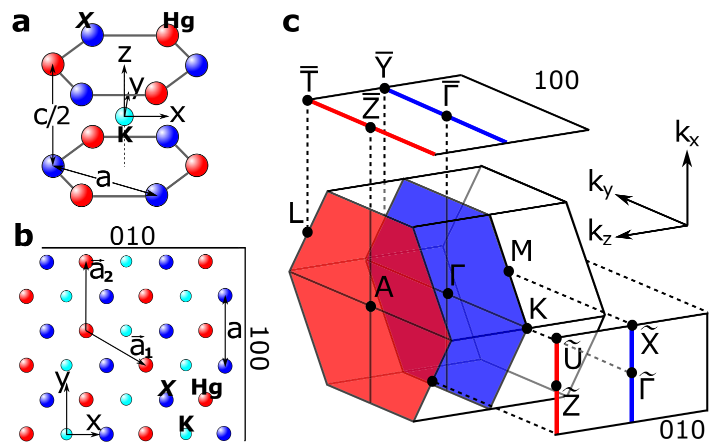




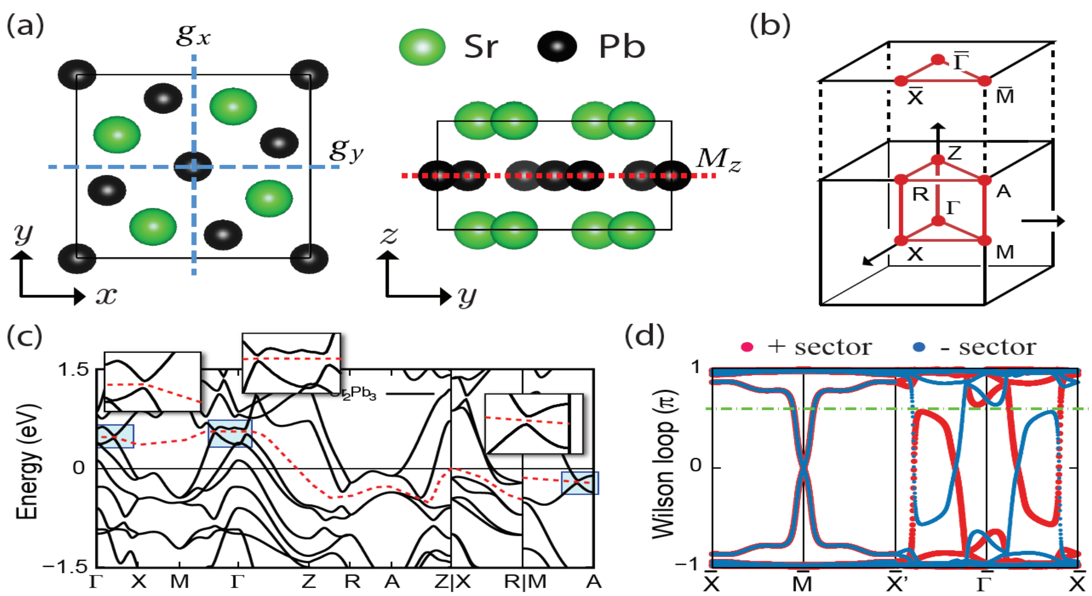
Topological Semimetals /
Weyl, Dirac and “beyond” Fermions
(3fold, 6fold and 8fold crossings)

NonSymmorphic Symmetries Bring In New Phenomena

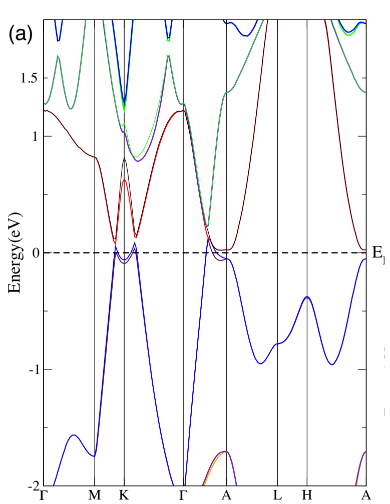


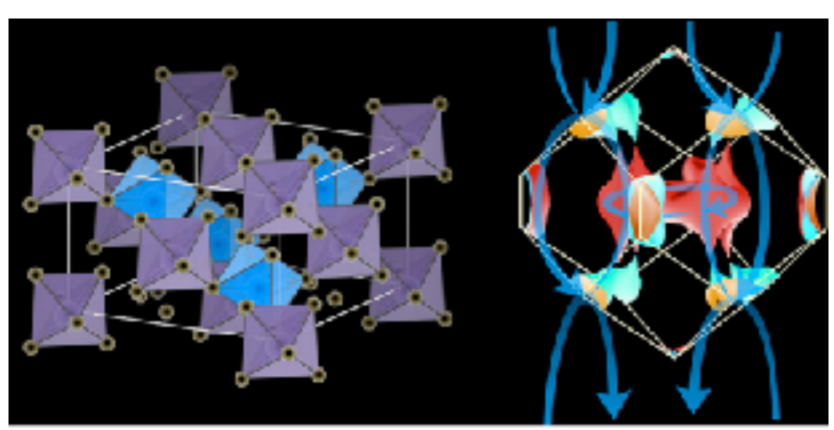


Surface States in KHgSb
One glide plane allows for the presence of
Hourglass-like fermions on the surface



Surface States in Sr2Pb3, a Dirac
Nonsymmorphic insulator
4-fold degeneracy surface state at the M
point with Two glide planes



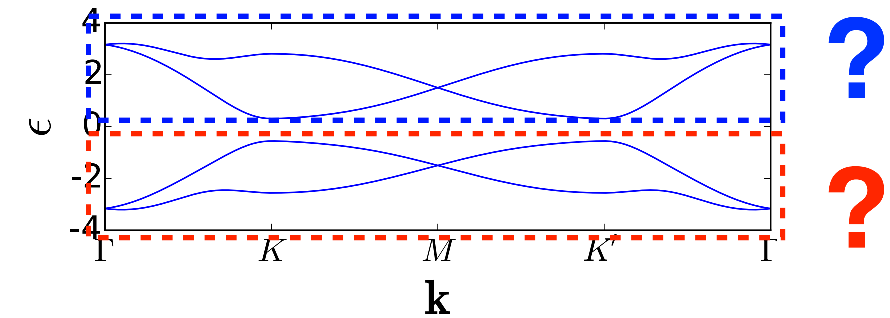


3,6,8-degeneracies (3 can also be realized
with symmorphic), nodal chains, etc

Non-predictive classification of Topological Bands

Open questions:

1. How do we know the classification is complete?



↕

Given an orbital content on a material on a lattice, what are the topological phases?

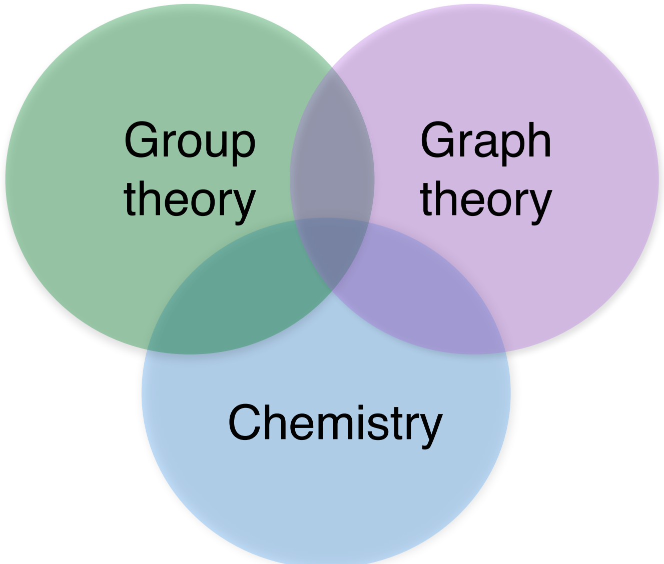
2. How can we find topological materials?

200000 materials in ICSD database:

100 time reversal topological insulators
10 mirror Chern insulators
15 Weyl semimetals
15 Dirac semimetals
3 Non-Symmorphic topological insulators

} Set of measure zero…
Are topological materials that esoteric?

We propose a classification that captures all crystal symmetries and has *predictive* power



Recall: a space group is a set of symmetries that defines a crystal structure in 3D

Ingredients:

230 Space-Groups {
- unit lattice translations ($\mathbb{Z}^3$)
- point group operations (rotations, reflections)
- non-symmorphic (screw, glide)
- orbitals
- atoms in some lattice positions

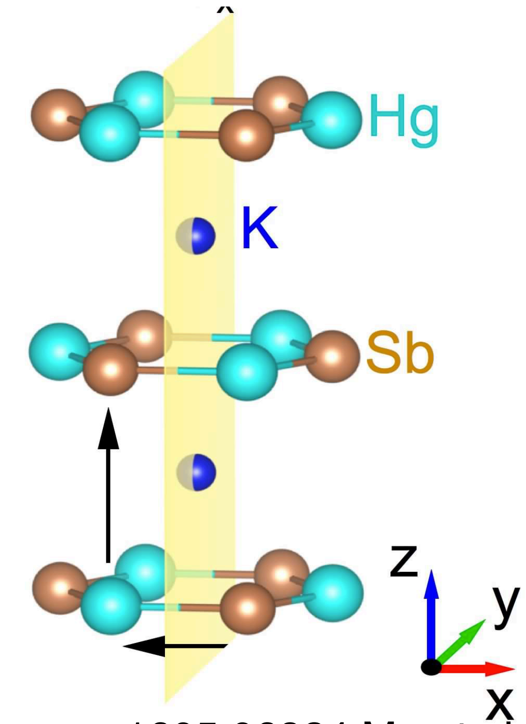


Image: 1605.06824 Ma et al

How do we go from real space orbitals sitting on lattice sites to electronic bands (without a Hamiltonian)?

ELEMENTARY BAND REPRESENATIONS

Zak PRB 26 (1982)

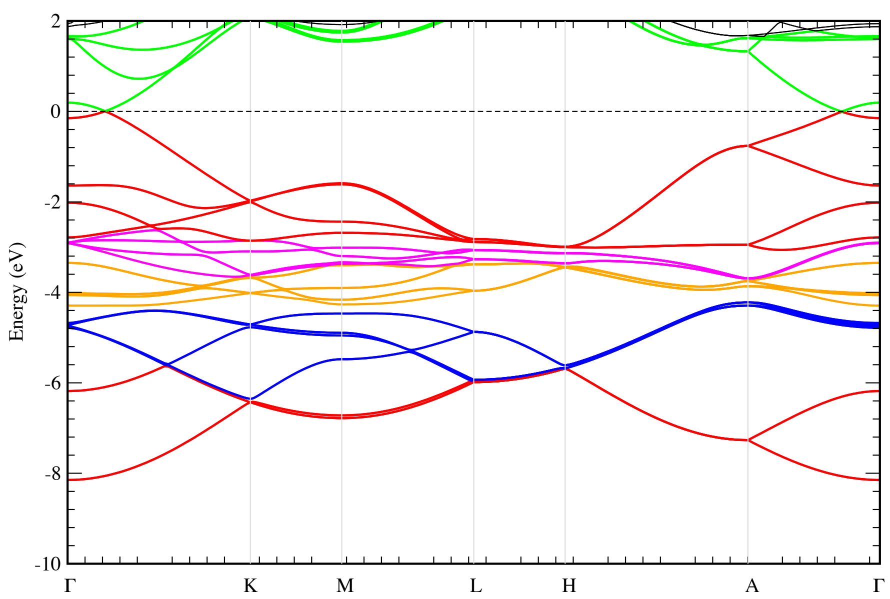
Elementary Band Representations (building blocks)

Band Representation (BR): set of bands linked to a localized orbital respecting all the crystal symmetries. They relate electrons on site to momentum space description.

↓

Elementary BR: smallest set of bands cannot be decomposed in elementary bands
Physical Elementary R: when EBR also respects TR symmetry
Composite BR: A BR which is not elementary is a "composite"

(P)EBRs are connected along the BZ

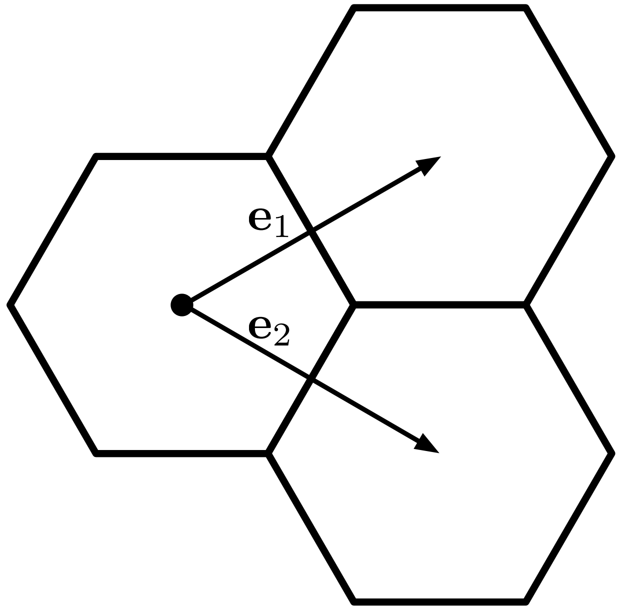


Zak PRB 26 (1982)

Induction of a (P)EBR: Example of the honeycomb lattice

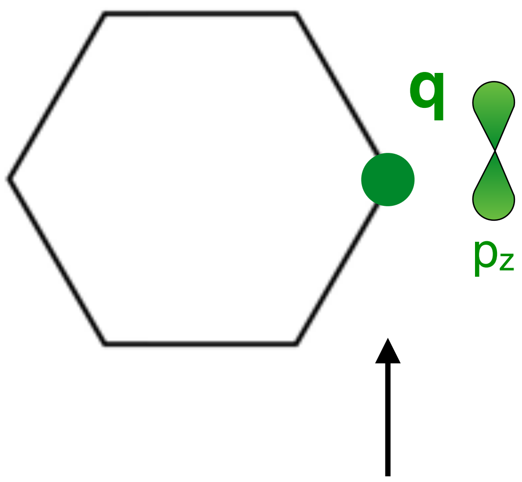
Lets consider the generators of 2D *P6mm*: $\{C_2, C_3, m_{1\bar{1}}\}$

Lattice vectors:



$$\begin{cases} \mathbf{e}_1 = \sqrt{3}/2\,\mathbf{x} + 1/2\,\mathbf{y} \\ \mathbf{e}_2 = \sqrt{3}/2\,\mathbf{x} - 1/2\,\mathbf{y} \end{cases}$$

Lattice site: Wyckoff 2b, spinfull p_z



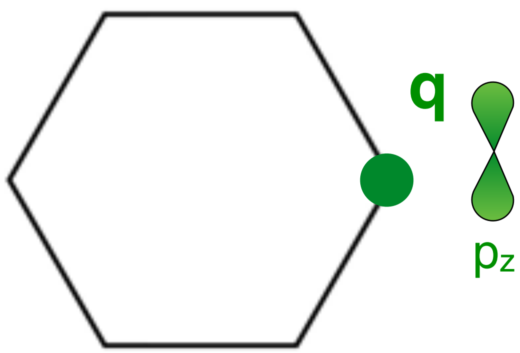
Site-symmetry group, $G_{\mathbf{q}}$, leaves **q** invariant

Cosset decomposition of a Space Group :

$$G = \bigcup_{\alpha=1}^{n} (g_\alpha)\,(G_q \ltimes \mathbb{Z}^3)\ ,\ g_\alpha \notin G_q$$

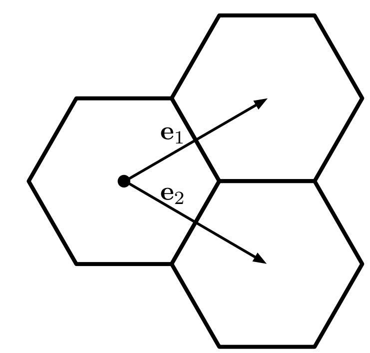
Induction of a (P)EBR: Example of the honeycomb lattice

Consider one lattice site:



$$G = \bigcup_{\alpha} (g_{\alpha})\ (G_q \ltimes \mathbb{Z}^3)$$

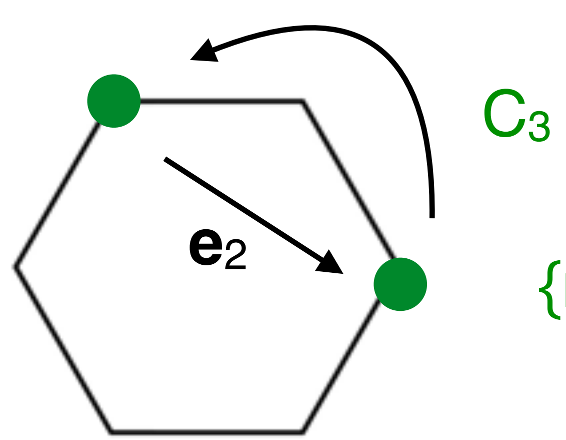
(2) (1)



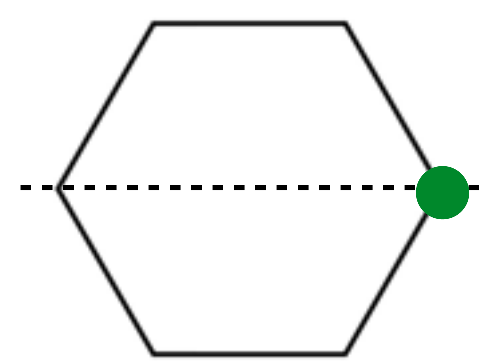
(1) Site-symmetry group, $G_{\mathbf{q}}$, leaves **q** invariant $\{C_3|01\}, \{m_{1\bar{1}}|00\} \approx C_{3v}$

→ Orbitals at **q** transform under a rep, ρ, of $G_{\mathbf{q}}$

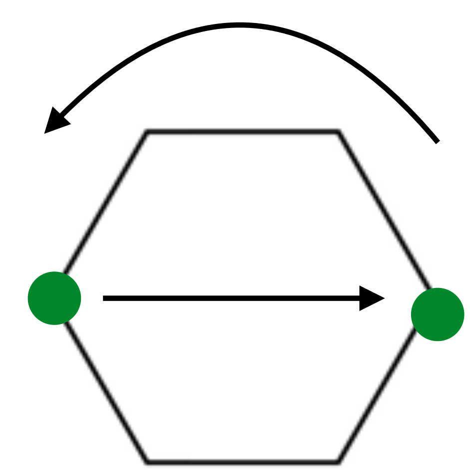
$\{C_3|01\}$



$\{m_{1\bar{1}}|00\}$

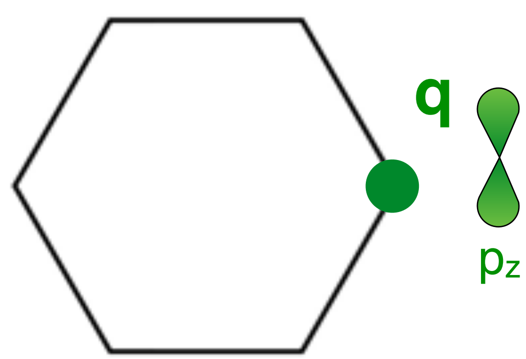


$\{C_2|?\}$



Induction of a (P)EBR: Example of the honeycomb lattice

Consider one lattice site:



$$G = \bigcup_{\boldsymbol{\alpha}} (g_{\boldsymbol{\alpha}})\ (G_q \ltimes \mathbf{Z}^3)$$

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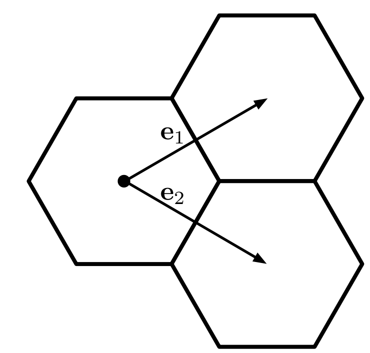

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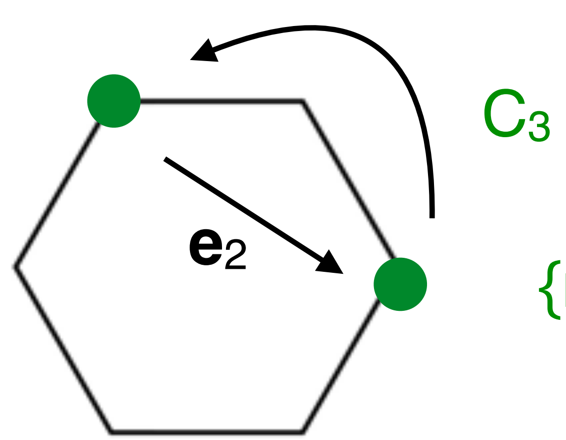
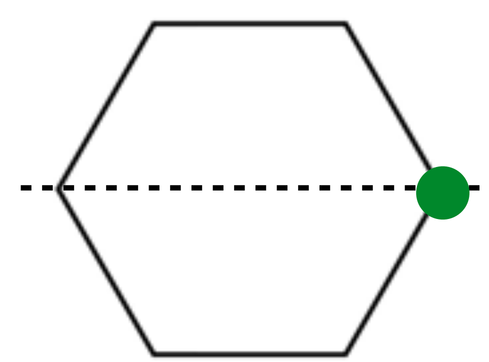
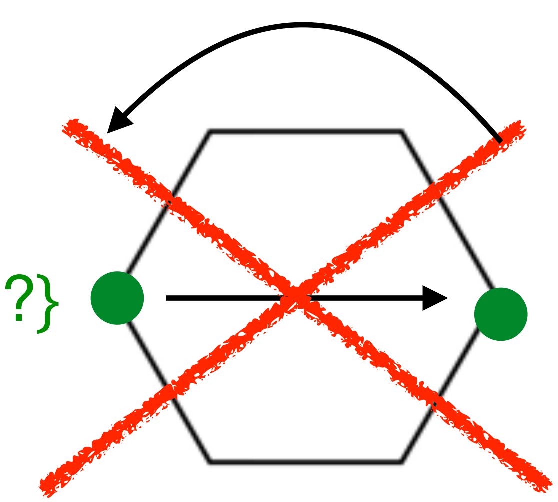


$\{m_{1\bar{1}}|00\}$

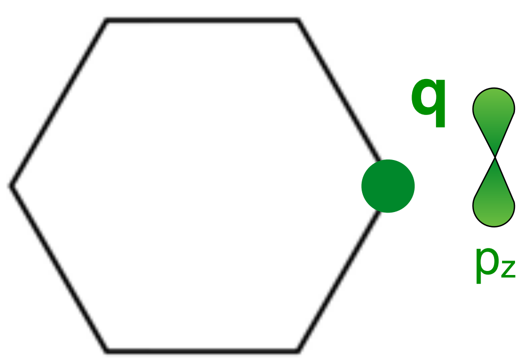


$\{C_2|?\}$



Induction of a (P)EBR: Example of the honeycomb lattice

Consider one lattice site:



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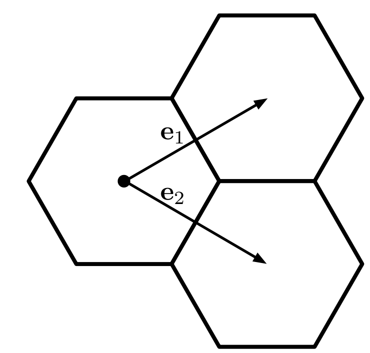
(2) (1)



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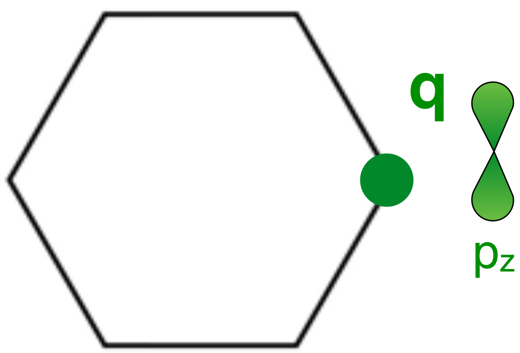
⟶ Orbitals at **q** transform under a rep, ρ, of $G_{\mathbf{q}}$

Rep	E	C_3	M	$\bar{E}$
⟶ $\bar{\Gamma}_6$	2	1	0	-2

Character table for the double-valued representation of C_{3v}

Induction of a (P)EBR: Example of the honeycomb lattice

Consider one lattice site:



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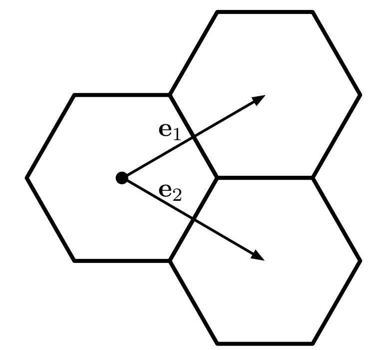

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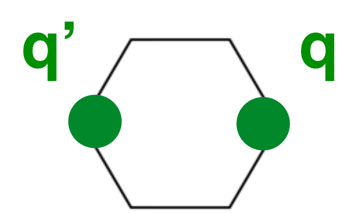
(2) Elements of space group $g \notin G_{\mathbf{q}}$ (cosset representatives) move sites in an orbit “Wyckoff position” $\{C_2|00\},\{E|00\}$

Wyckoff multiplicity: 2
orbit of q



Induction of a (P)EBR: Example of the honeycomb lattice

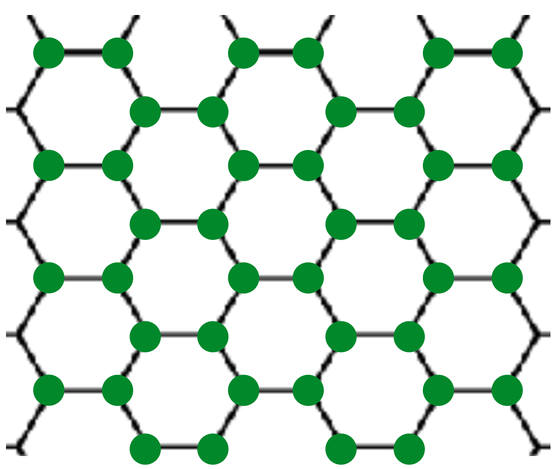
$\bar{\Gamma}_6$ induced in C_{6v}

electron bands sitting at pz orbitals in
Wyckoff 2b in Wall paper group 17

$$\rho_G = \rho \uparrow G$$

Cosset representative g: {C_2I00},{EI00}

h ∊ G, generators of
honeycomb lattice: C_2,C_3,σ



$$\rho_{i\alpha,j\beta}(h) = \rho_{ij}(g_{\alpha\beta})$$

$$g_{\alpha\beta} = g_\alpha^{-1}\{E|t_{\alpha\beta}\}hg_\beta$$

$$\rho_G^{\mathbf{k}}(h) = e^{-(\mathbf{k}\cdot t_{\alpha\beta})}\rho_{ij}(g_{\alpha\beta})$$

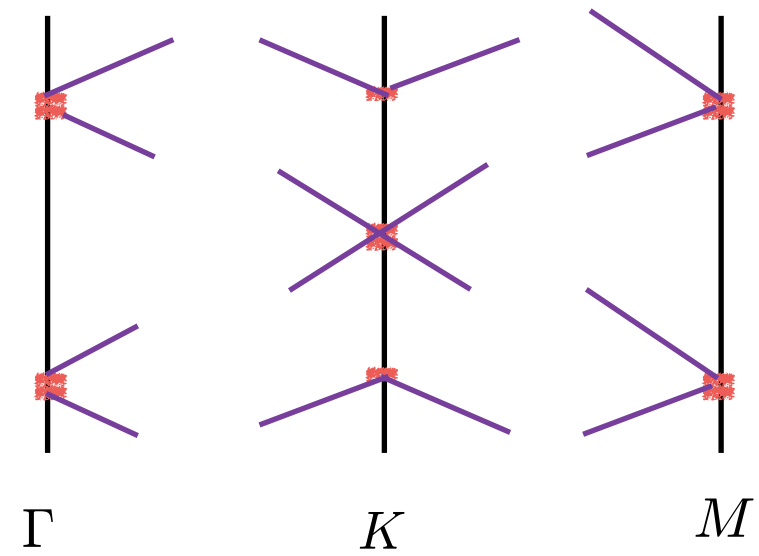
dimension of this band representations = connectivity in the Brillouin zone

Subduction in k space: IRREPS at points, lines

Restricting to the little group at k to find irreps at each k point (subduction) -> **all bands connected**

All 10403 decompositions now tabulated on the Bilbao Crystallographic Server

$(\rho \uparrow G) \downarrow G_k$

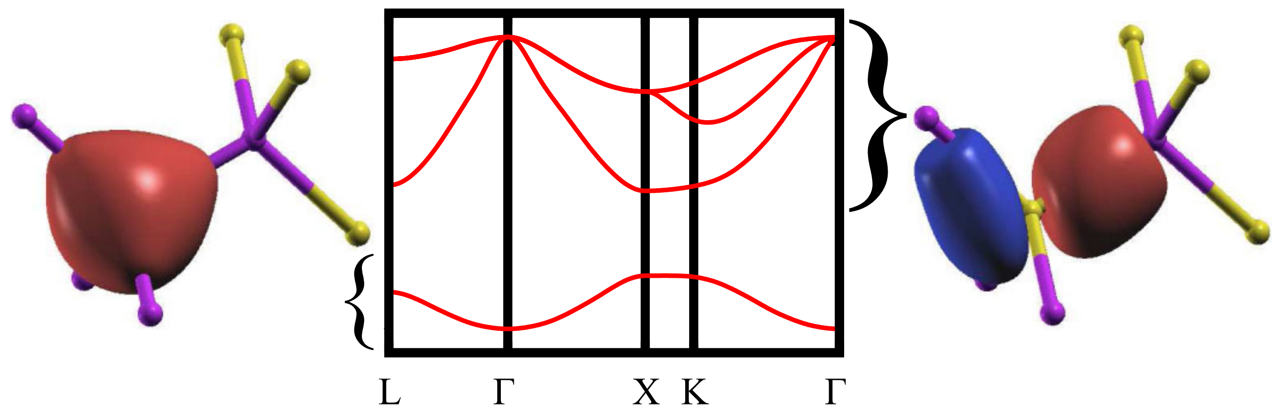


By construction, a band representation has an atomic limit, and all atomic limits yield a band representation

↕

Recall: Topological bands CANNOT Have Maximally Localized Wannier Functions…

Why are Elementary Band Representations Important?



1) Bands in ρ_G are connected (this phase can always realized) in the Brillouin zone

2) Bands in ρ_G are not connected: at least one topological band

Disconnected (P)EBR = set of disconnected bands that connected form an (P)EBR

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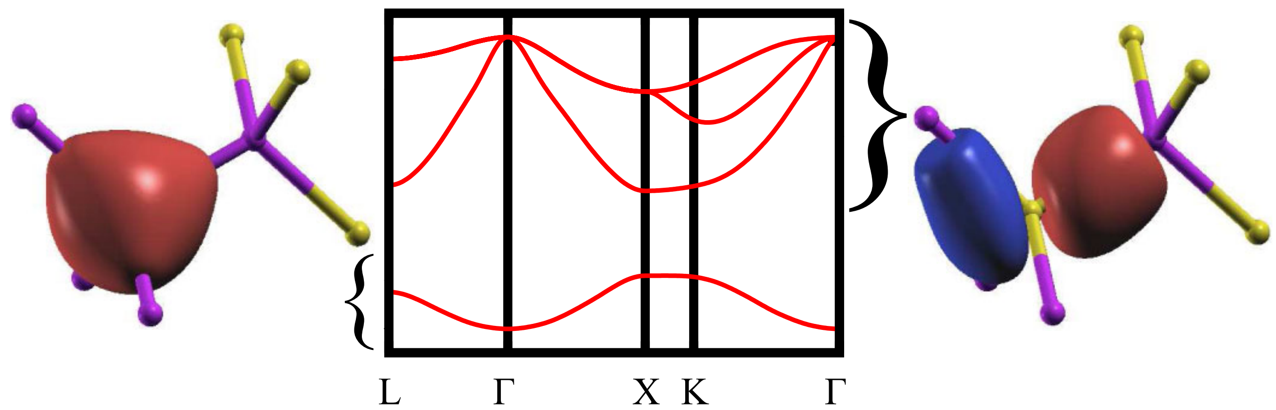

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Disconnected (P)EBR = set of disconnected bands that connected form an (P)EBR

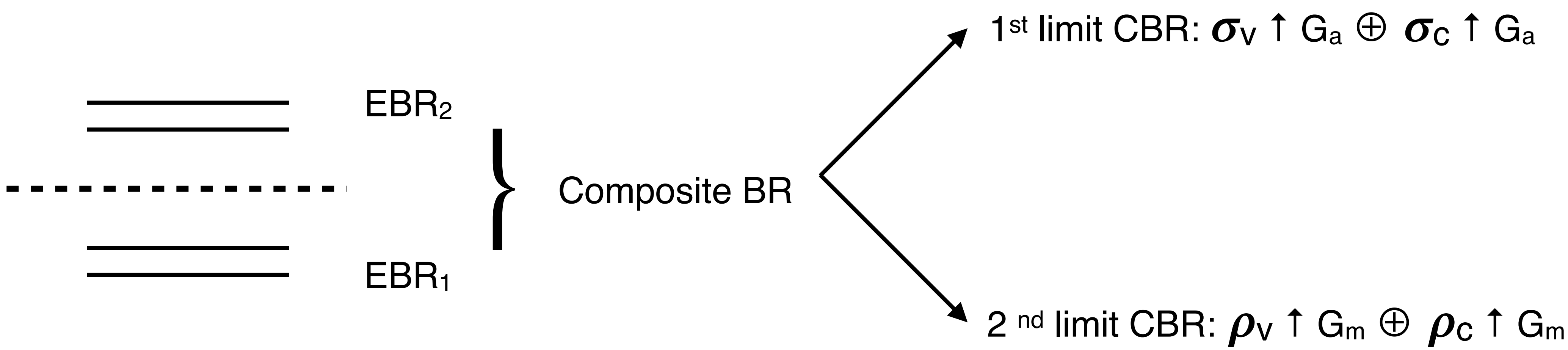
Our definition of a **topological band** = anything that is **not a band representation**

Obstructed atomic limit

Orbital hybridization

BR are induced from localized molecular orbitals, away from the atoms

In terms of EBRs?



1^{st} limit: orbitals lie in the atomic sites

2^{nd} limit: orbitals do not coincide with the atoms

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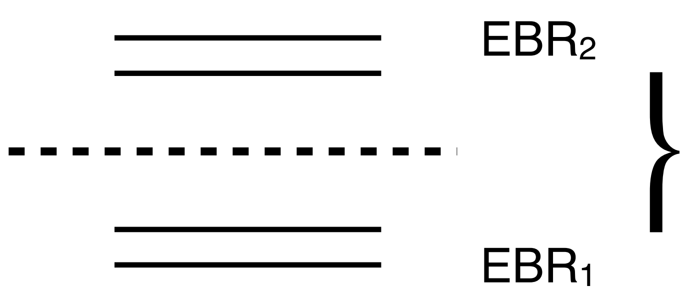


Composite BR

1st limit CBR: $\boldsymbol{\sigma}_V \uparrow G_a \oplus \boldsymbol{\sigma}_C \uparrow G_a$

$\eta \uparrow G_a \approx \boldsymbol{\sigma}_V \oplus \boldsymbol{\sigma}_C$

$\eta \uparrow G_m \approx \boldsymbol{\rho}_V \oplus \boldsymbol{\rho}_C$

2 nd limit CBR: $\boldsymbol{\rho}_V \uparrow G_m \oplus \boldsymbol{\rho}_C \uparrow G_m$

1st limit: orbitals lie in the atomic sites

2 nd limit: orbitals do not coincide with the atoms

This is a “chemical bonding” transition (ex: from week to a strong covalent bonding)

N. Read Phys.Rev. B (2017), W. A. Benalcazar Science (2017)

TQC statement

All sets of bands induced from symmetric, localized orbitals, are topologically trivial by design.

Zak PRB 26 (1982)

TQC statement

NOT

All sets of bands induced from symmetric, localized orbitals, are topologically trivial by design.

NOT

Zak PRB 26 (1982)

Elementary Band Representations (reciprocal space)

Global information about band structure: enumerate all EBRs

1. Maximal k-vectors and path
2. Compatibility relations
3. Graph theory: identification of disconnected bands

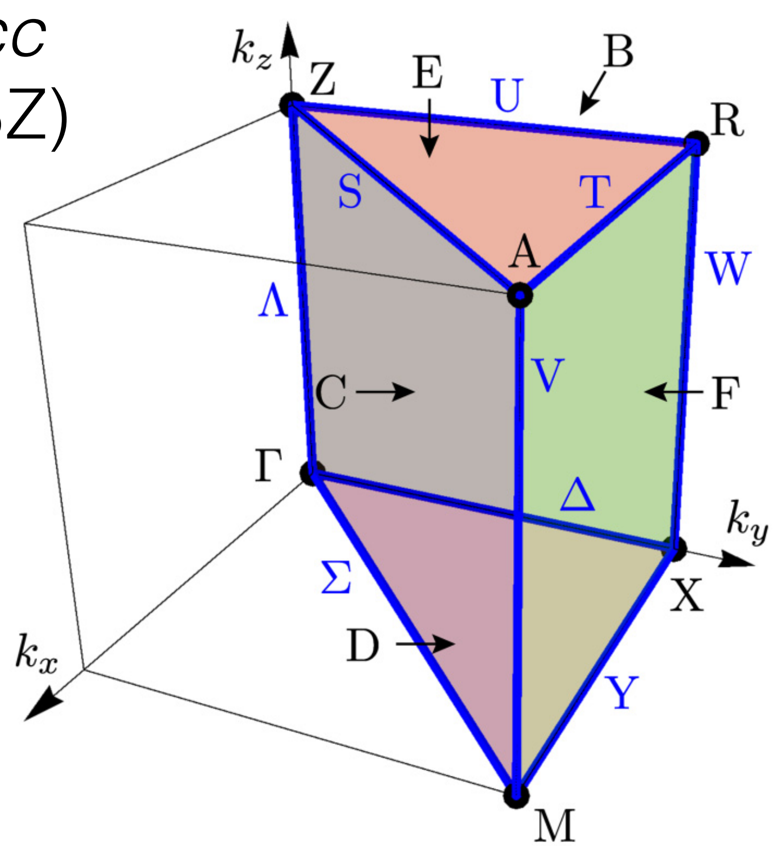
Zak PRB 26 (1982)

1. Maximal k-vectors and paths

For all the 203 SG:
maximal k-vectors + minimal set non-redundant **connections**

(1) **k** vector in a manifold is maximal if its little co-group it's not a subgroup of another manifold of vectors **k'** (in general coincides with high-symmetry k-vector)

P4/ncc
(first BZ)



k-vec	mult.	Coordinates	Little	Maximal co-group	TR
Γ	1	(0,0,0)	$4/mmm(D_{4h})$	yes	yes
Z	1	(0,0,1/2)	$4/mmm(D_{4h})$	yes	yes
M	1	(1/2,1/2,0)	$4/mmm(D_{4h})$	yes	yes
A	1	(1/2,1/2,1/2)	$4/mmm(D_{4h})$	yes	yes
R	2	(0,1/2,1/2)	$mmm(D_{2h})$	yes	yes
X	2	(0,1/2,0)	$mmm(D_{2h})$	yes	yes
Λ	2	$(0,0,w), 0 < w < 1/2$	$4mm(C_{4v})$	no	no
V	2	$(1/2,1/2,w), 0 < w < 1/2$	$4mm(C_{4v})$	no	no
W	4	$(0,1/2,w), 0 < w < 1/2$	$mm2(C_{2v})$	no	no
Σ	4	$(u,u,0), 0 < u < 1/2$	$mm2(C_{2v})$	no	no
S	4	$(u,u,1/2), 0 < u < 1/2$	$mm2(C_{2v})$	no	no
Δ	4	$(0,v,0), 0 < v < 1/2$	$mm2(C_{2v})$	no	no
U	4	$(0,v,1/2), 0 < v < 1/2$	$mm2(C_{2v})$	no	no
Y	4	$(u,1/2,0), 0 < u < 1/2$	$mm2(C_{2v})$	no	no
T	4	$(u,1/2,1/2), 0 < u < 1/2$	$mm2(C_{2v})$	no	no
D	8	$(u,v,0), 0 < u < v < 1/2$	$m(C_s)$	no	no
E	8	$(u,v,1/2), 0 < u < v < 1/2$	$m(C_s)$	no	no
C	8	$(u,u,w), 0 < u < w < 1/2$	$m(C_s)$	no	no
B	8	$(0,v,w), 0 < v < w < 1/2$	$m(C_s)$	no	no
F	8	$(u,1/2,w), 0 < u < w < 1/2$	$m(C_s)$	no	no
GP	16	$(u,v,w), 0 < u < v < w < 1/2$	1(1)	no	no

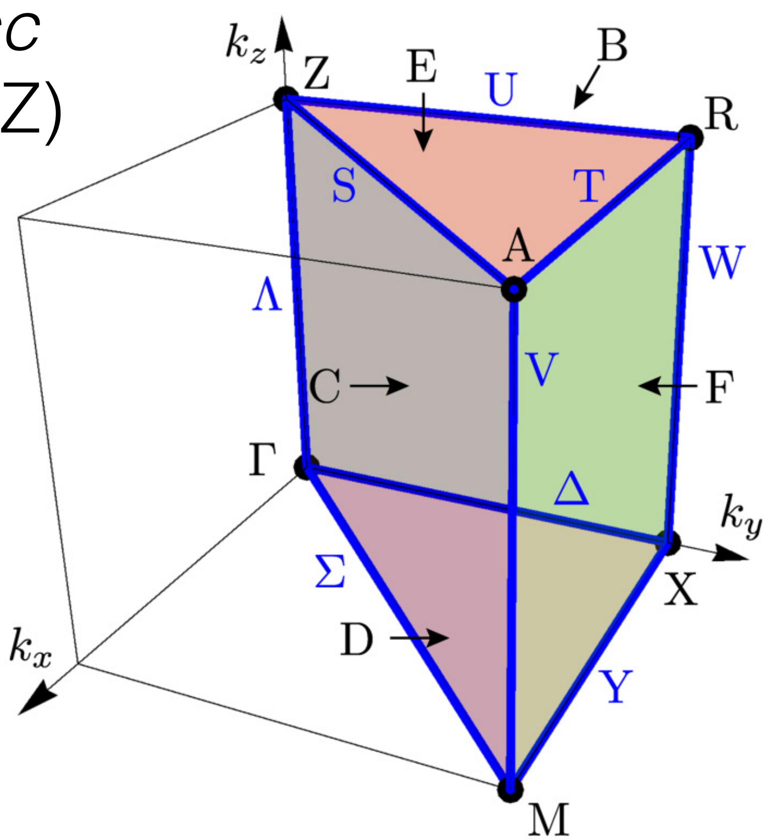
Physical Review E 96 (2), 023310

1. Maximal k-vectors and paths

For all the 203 SG:
maximal k-vectors + minimal set non-redundant **connections**

(1) **k** vector in a manifold is maximal if its little co-group it's not a subgroup of another manifold of vectors **k'** (in general coincides with high-symmetry k-vector)

P4/ncc
(first BZ)



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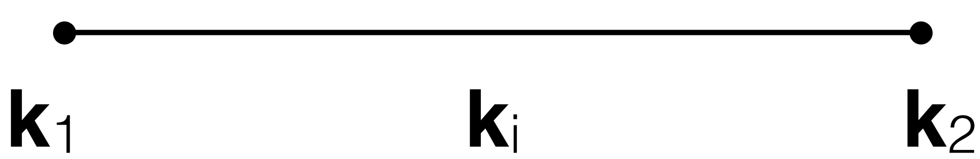
A	1	(1/2,1/2,1/2)	$4/mmm(D_{4h})$	yes	yes
R	2	(0,1/2,1/2)	$mmm(D_{2h})$	yes	yes
X	2	(0,1/2,0)	$mmm(D_{2h})$	yes	yes
Λ	2	$(0,0,w),0 < w < 1/2$	$4mm(C_{4v})$	no	no
V	2	$(1/2,1/2,w),0 < w < 1/2$	$4mm(C_{4v})$	no	no
W	4	$(0,1/2,w),0 < w < 1/2$	$mm2(C_{2v})$	no	no
Σ	4	$(u,u,0),0 < u < 1/2$	$mm2(C_{2v})$	no	no
S	4	$(u,u,1/2),0 < u < 1/2$	$mm2(C_{2v})$	no	no
Δ	4	$(0,v,0),0 < v < 1/2$	$mm2(C_{2v})$	no	no
U	4	$(0,v,1/2),0 < v < 1/2$	$mm2(C_{2v})$	no	no
Y	4	$(u,1/2,0),0 < u < 1/2$	$mm2(C_{2v})$	no	no
T	4	$(u,1/2,1/2),0 < u < 1/2$	$mm2(C_{2v})$	no	no
D	8	$(u,v,0),0 < u < v < 1/2$	$m(C_s)$	no	no
E	8	$(u,v,1/2),0 < u < v < 1/2$	$m(C_s)$	no	no
C	8	$(u,u,w),0 < u < w < 1/2$	$m(C_s)$	no	no
B	8	$(0,v,w),0 < v < w < 1/2$	$m(C_s)$	no	no
F	8	$(u,1/2,w),0 < u < w < 1/2$	$m(C_s)$	no	no
GP	16	$(u,v,w),0 < u < v < w < 1/2$	1(1)	no	no

1. Maximal k-vectors and paths

(2) All possible connection between maximal and non-maximal **k**-vectors

→ 2 manifolds are connected if:

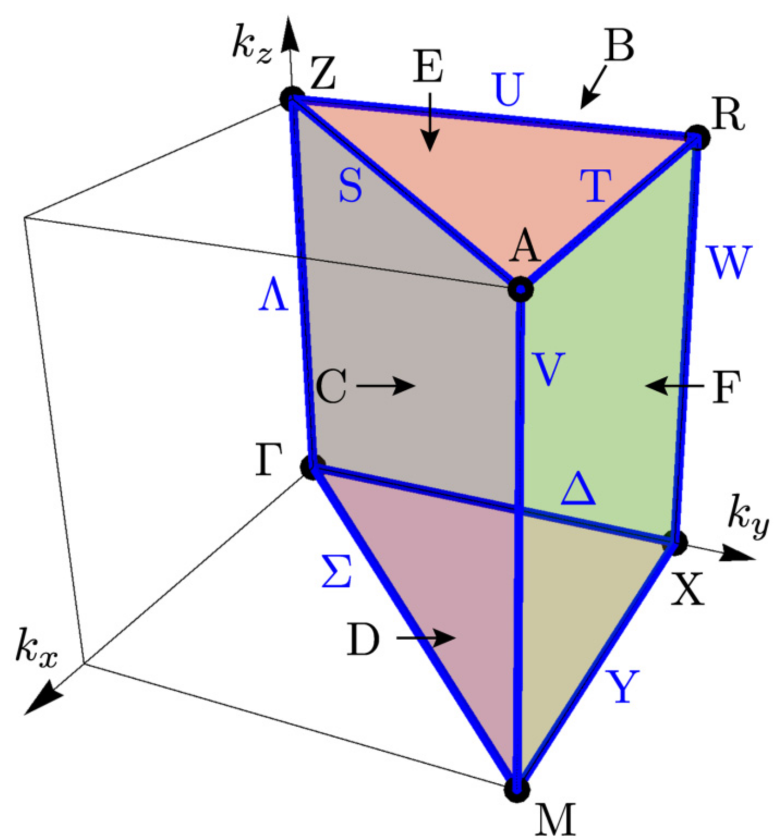


$\mathbf{k}_i(\mathbf{u}_1)=\mathbf{k}_1$

$\mathbf{k}_i(\mathbf{u}_2)=\mathbf{k}_2$

for each max. **k** in ***k** and $\mathbf{k}_i$ non-maximal

P4/ncc
(first BZ)

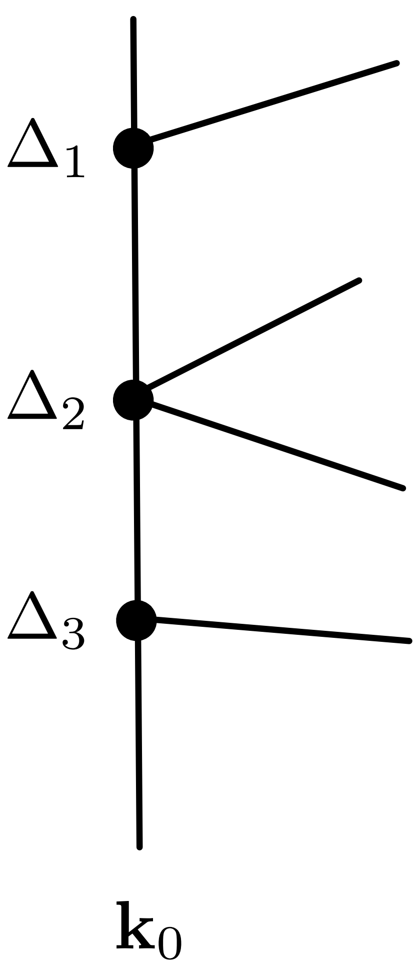


Maximal **k**-vec	Connected **k**-vecs	Specific coordinates	Connections with the star
Γ: (0,0,0)	Λ: $(0,0,w)$	$w=0$	2
	Δ: $(0,v,0)$	$v=0$	4
	Σ: $(u,u,0)$	$u=0$	4
	B: $(0,v,w)$	$v=w=0$	8
	C: (u,u,w)	$u=w=0$	8
	D: $(u,v,0)$	$u=v=0$	8

Γ:3 lines and 3 planes

2. Compatibility Relations

Is the way in which both the point group symmetry and the translational symmetry of the crystal lattice are incorporated into the formalism that describes elementary excitations in a solid.



- Bloch Hamiltonian is constrained by symmetry

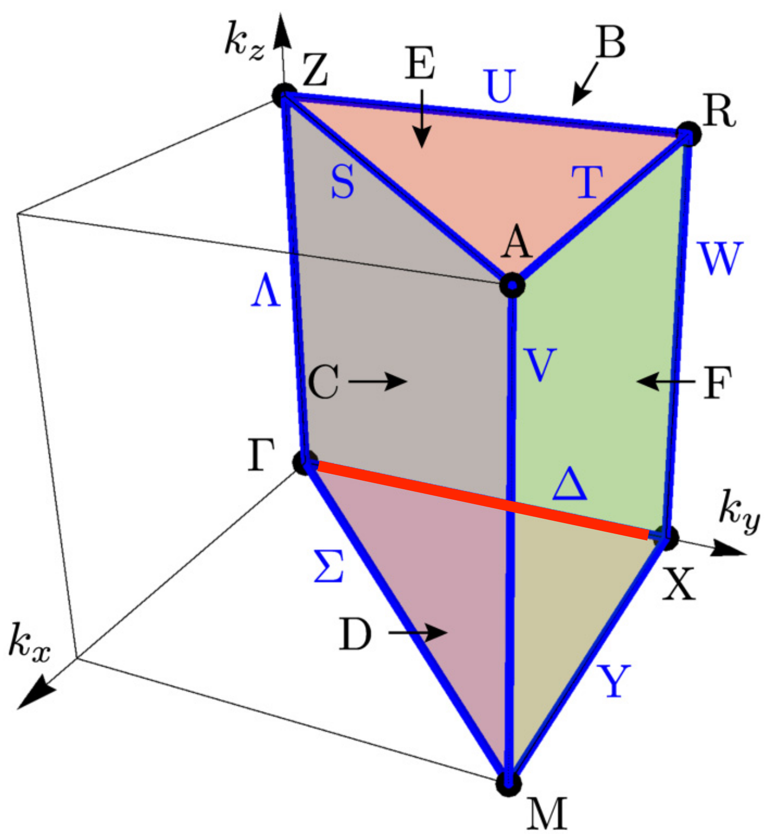
$$\Delta(\mathcal{G})H(\mathbf{k})\Delta(\mathcal{G})^{-1} = H(\mathcal{G}\mathbf{k})$$

- At high symmetry points $\mathbf{k_0}$, Bloch functions are classified by IRREPS

$$\delta\mathbf{k} = \mathbf{k} - \mathbf{k}_0 \longrightarrow H(\mathbf{k}) \approx \bigoplus_{\text{irreps}} H_{\Delta_{\mathbf{k}_0}}(\mathbf{k})$$

- Compatibility relations tell us how the different $\mathbf{k}\cdot\mathbf{p}$ hamiltonians are connected

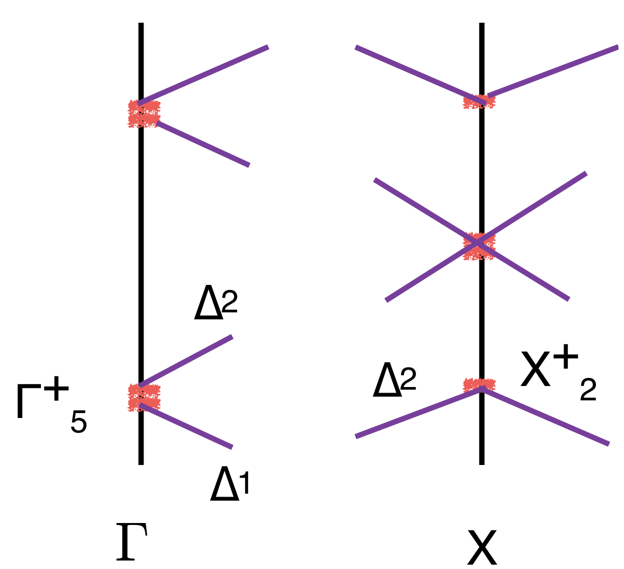
2. Compatibility Relations



- Let's consider 2 high symmetry points of the SG 130 : Γ and X
  1. symmetry operations point group Γ (k_1) are the ones of O_h
  2. symmetry operations point group X (k_2) are the ones of D_{4h}
- Both high symmetry points are connected through Δ (k_t) with C_{4v}
- In general

$$(\Gamma\ (k_1)):\ \rho \downarrow G_{\mathbf{k}_t} \approx \bigoplus_i \tau_i \quad \text{and} \quad (X\ (k_2)):\ \sigma \downarrow G_{\mathbf{k}_t} \approx \bigoplus_i \tau_i$$

Example:



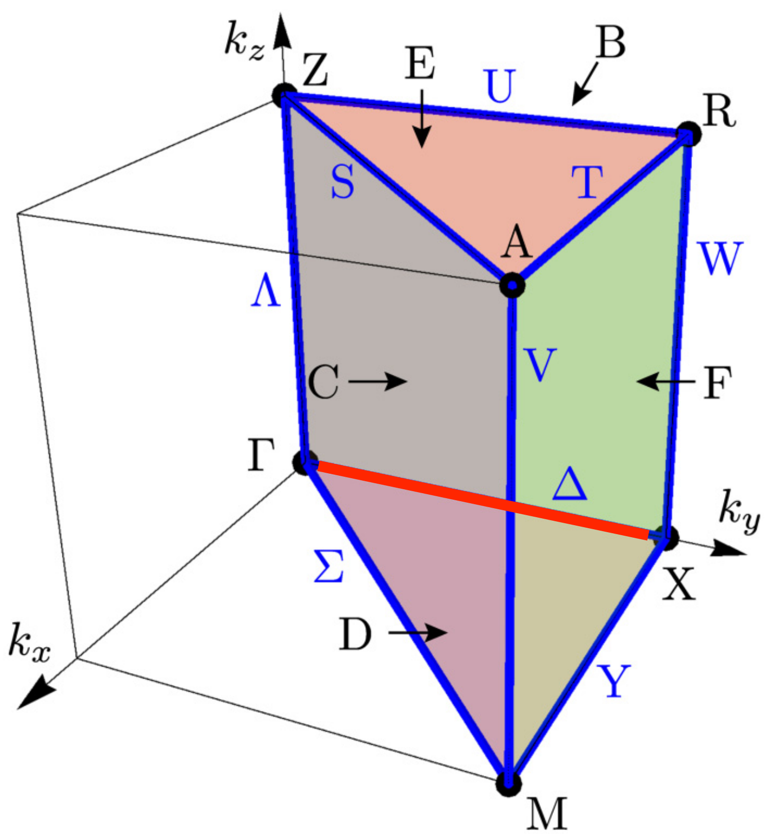
Γ^+_5 of O_h is a reducible representation of C_{4v}

↓

Reduction of Γ^+_5 into irreducible representations of C_{4v} yields the compatibility relation

$$\Gamma^+_5 \rightarrow \Delta_1 + \Delta_2$$

2. Compatibility Relations



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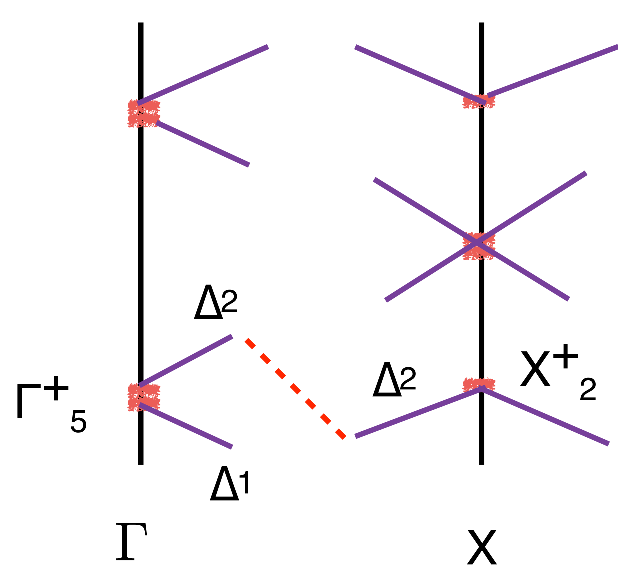
Example:



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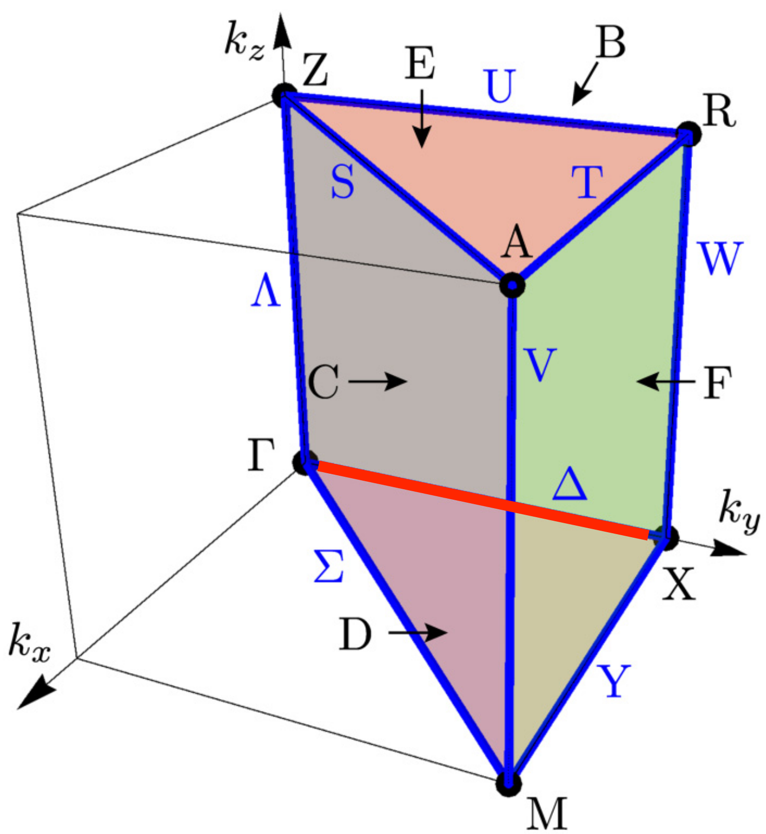

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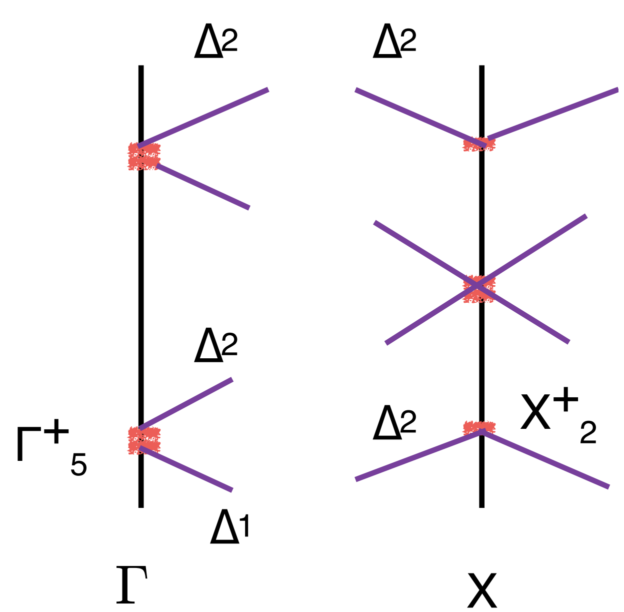

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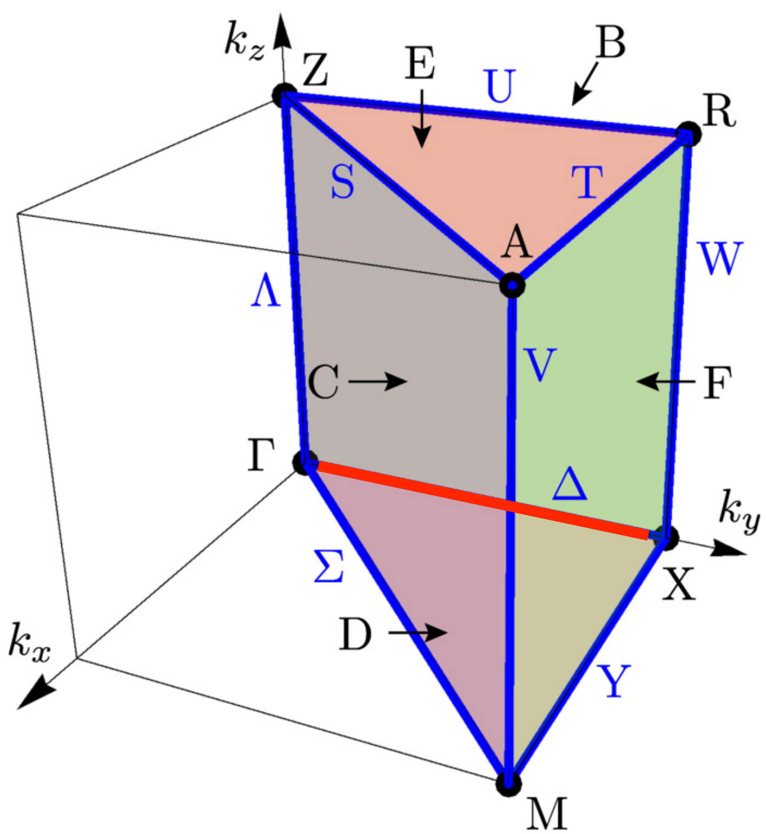
2. Compatibility Relations



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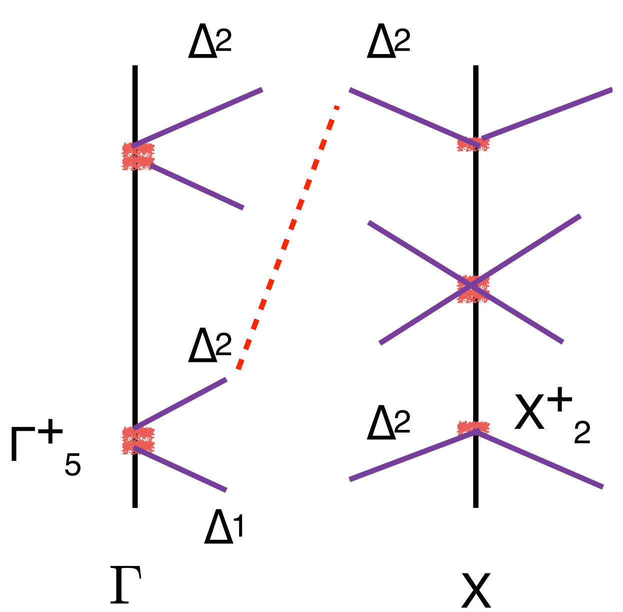

$\Gamma^+{}_5$ of O_h is a reducible representation of C_{4v}

↓

Reduction of $\Gamma^+{}_5$ into irreducible representations of C_{4v} yields the compatibility relation

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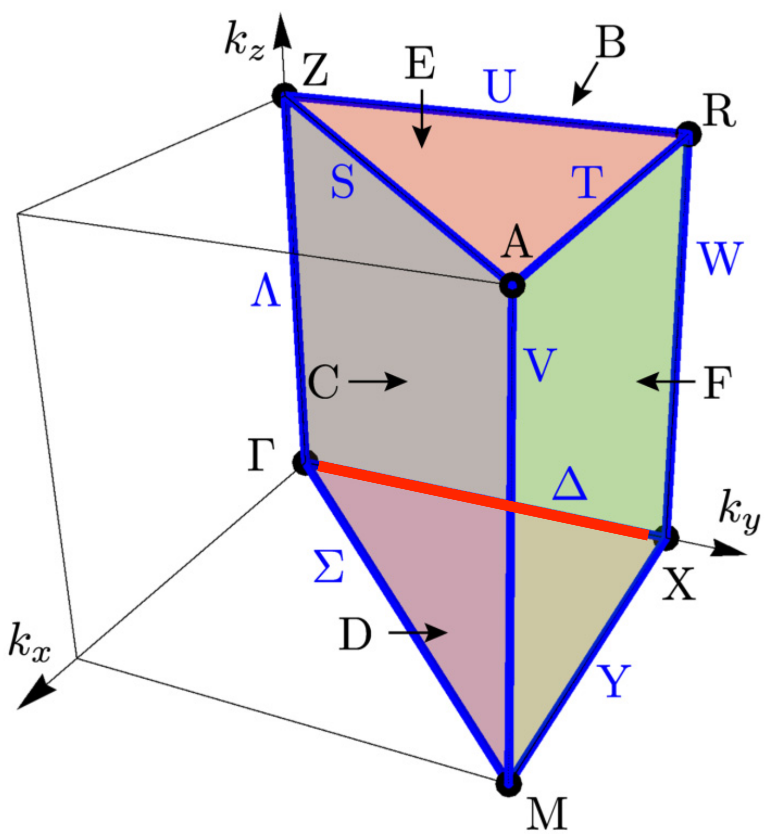
2. Compatibility Relations



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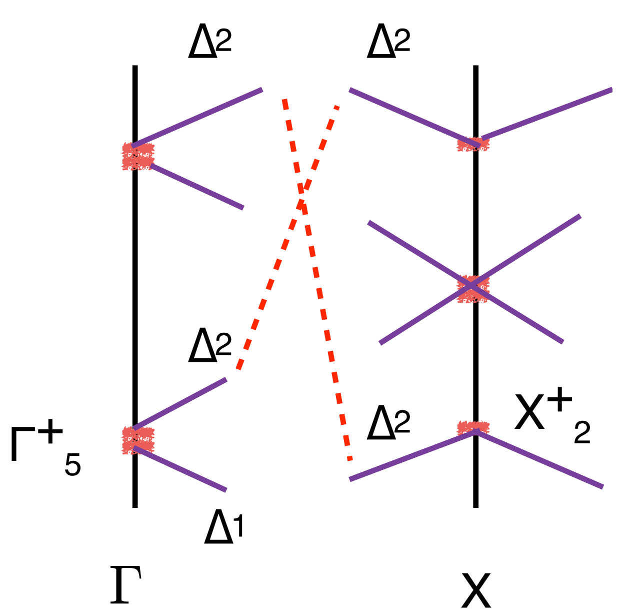

Γ^+_5 of O_h is a reducible representation of C_{4v}

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Reduction of Γ^+_5 into irreducible representations of C_{4v} yields the compatibility relation

$$\Gamma^+_5 \rightarrow \Delta_1 + \Delta_2$$

2. Compatibility Relations

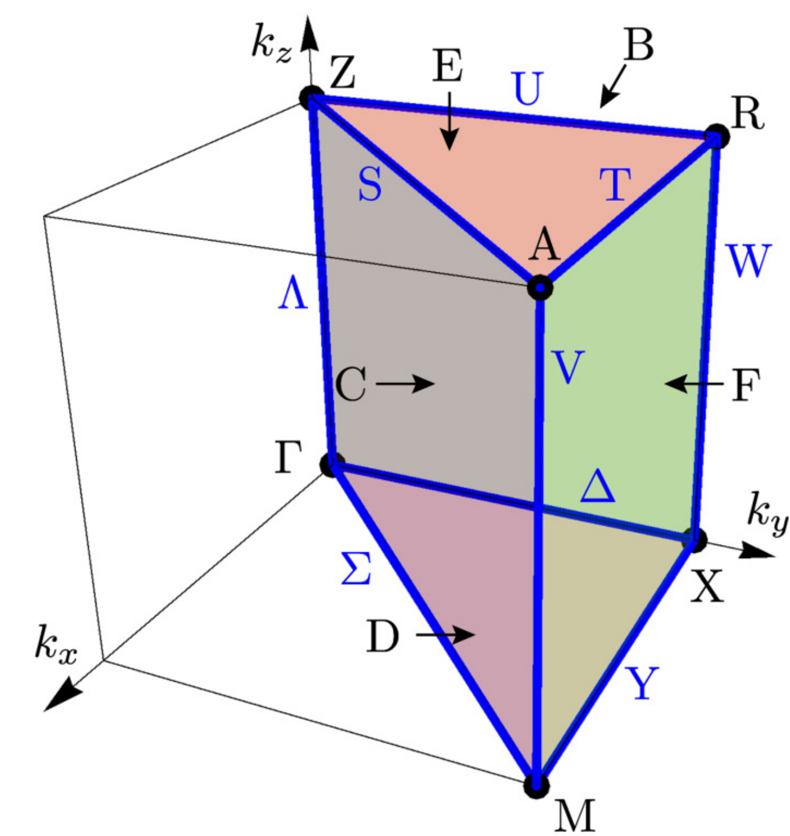
Reducing the number of paths

(i) Paths are subspace of other paths
k^1_M and k^2_M connect through k_p and k_l, k_p is redundant

(ii) Paths related by symmetry operations
A single line or plane of the *k gives all independent restrictions

(iii) Paths that are combinations of other paths

* additional restrictions in non-symmorphic groups (monodromy)

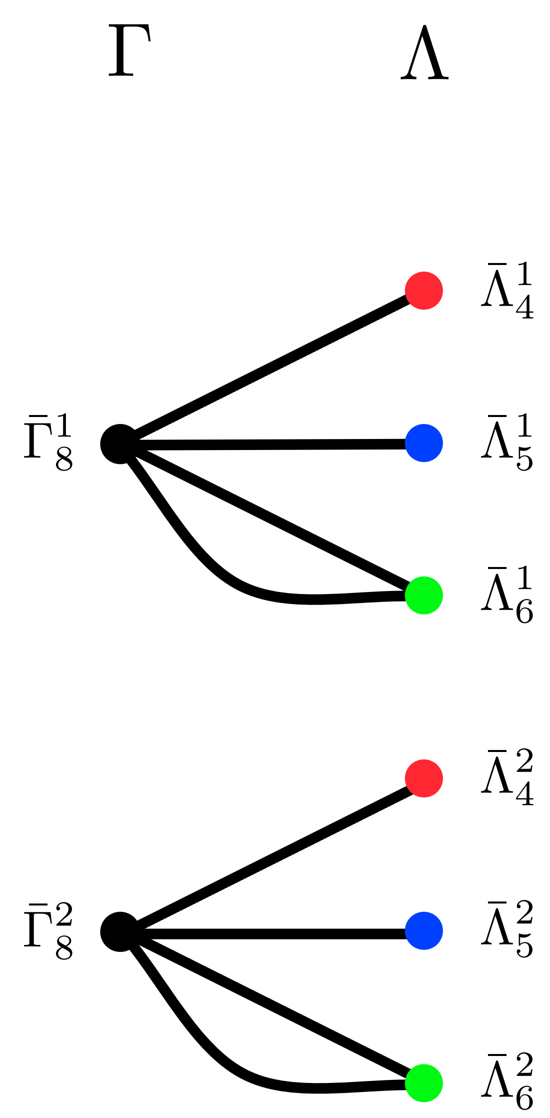


3. Connectivity graphs
(honeycomb lattice)

- We must ensure compatibility relations are satisfied along the lines and planes joining little groups
- There will be many ways to form energy bands, consisten with compatibility relations
- **Goal: classify the valid band structures**
- We can accomplish this introducing a graph-theory picture

↓

Partition: High symmetry point
Nodes: irreps of the little group
Graph connectivity: Band connectivity problem



3. Connectivity graphs

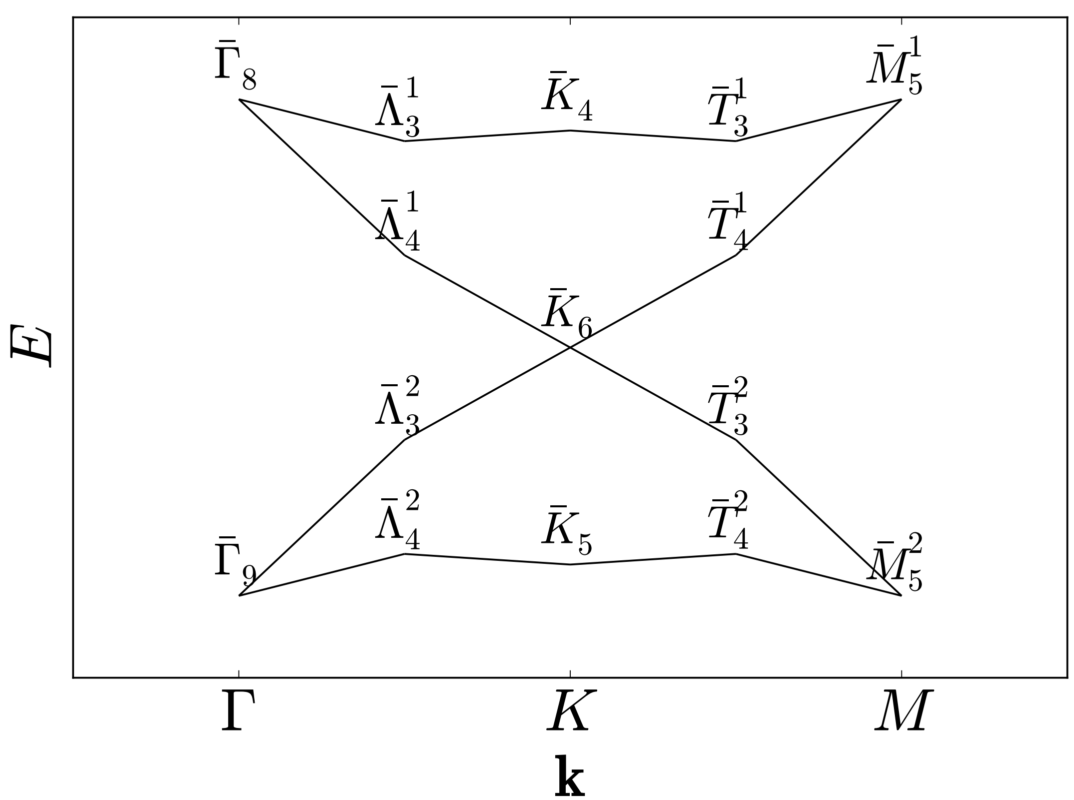
Adjacency matrix: *m x m* matrix, where the (ij)'th entry is the number of edge connection i to j
Degree matrix: diagonal matrix is whose (ii)'th entry is the degree of the node i
Laplacian matrix: L= A-D

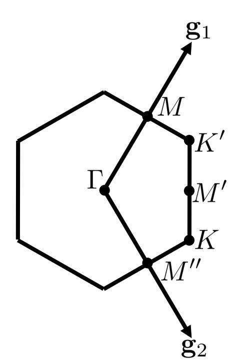
$$
A_1 = \begin{array}{c}
\begin{array}{ccccccccccccccccccc}
\bar\Gamma_8 & \bar\Gamma_9 & \bar\Sigma_3^1 & \bar\Sigma_3^2 & \bar\Sigma_4^1 & \bar\Sigma_4^2 & \bar\Lambda_3^1 & \bar\Lambda_3^2 & \bar\Lambda_4^1 & \bar\Lambda_4^2 & \bar K_4 & \bar K_5 & \bar K_6 & \bar T_3^1 & \bar T_3^2 & \bar T_4^1 & \bar T_4^2 & \bar M_5^1 & \bar M_5^2
\end{array} \\
\left(\begin{array}{cc|cccc|cccc|ccc|cccc|cc}
0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\hline
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\hline
0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0
\end{array}\right)
\begin{array}{c}
\bar\Gamma_8 \\ \bar\Gamma_9 \\ \bar\Sigma_3^1 \\ \bar\Sigma_3^2 \\ \bar\Sigma_4^1 \\ \bar\Sigma_4^2 \\ \bar\Lambda_3^1 \\ \bar\Lambda_3^2 \\ \bar\Lambda_4^1 \\ \bar\Lambda_4^2 \\ \bar K_4 \\ \bar K_5 \\ \bar K_6 \\ \bar T_3^1 \\ \bar T_3^2 \\ \bar T_4^1 \\ \bar T_4^2 \\ \bar M_5^1 \\ \bar M_5^2
\end{array}
\end{array}
$$

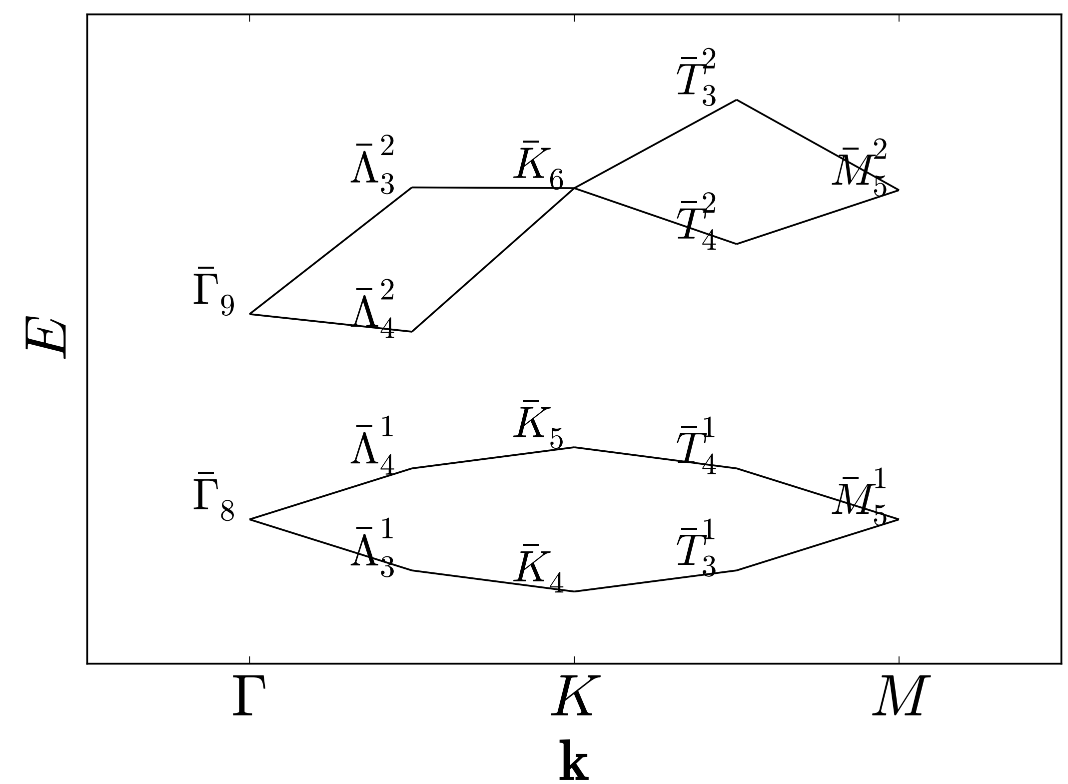
For each connected component of a graph, there is a 0 eigenvector of the Laplacian

Results: Graphene

2 independent Adjacency matrices:







- Single connected component
→ Fully connected and protected semi-metallic phase

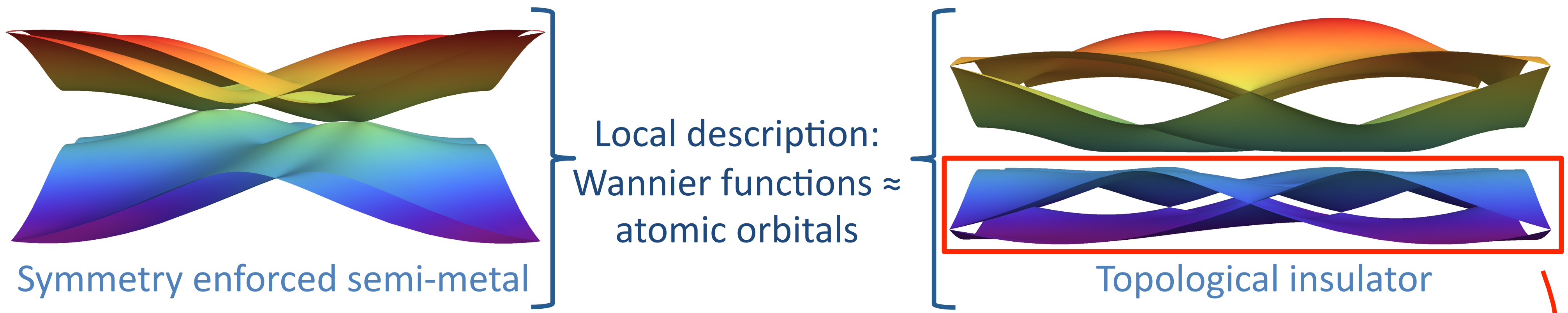
- Splitting of EBR
→ Topological bands

Vanderbilt, Soluyanov PRB 83, 035108 (2011)

Results: Graphene

What makes the disconnected bands topological?

All four bands come from a single set of localized orbitals (p_z, spin up/down)

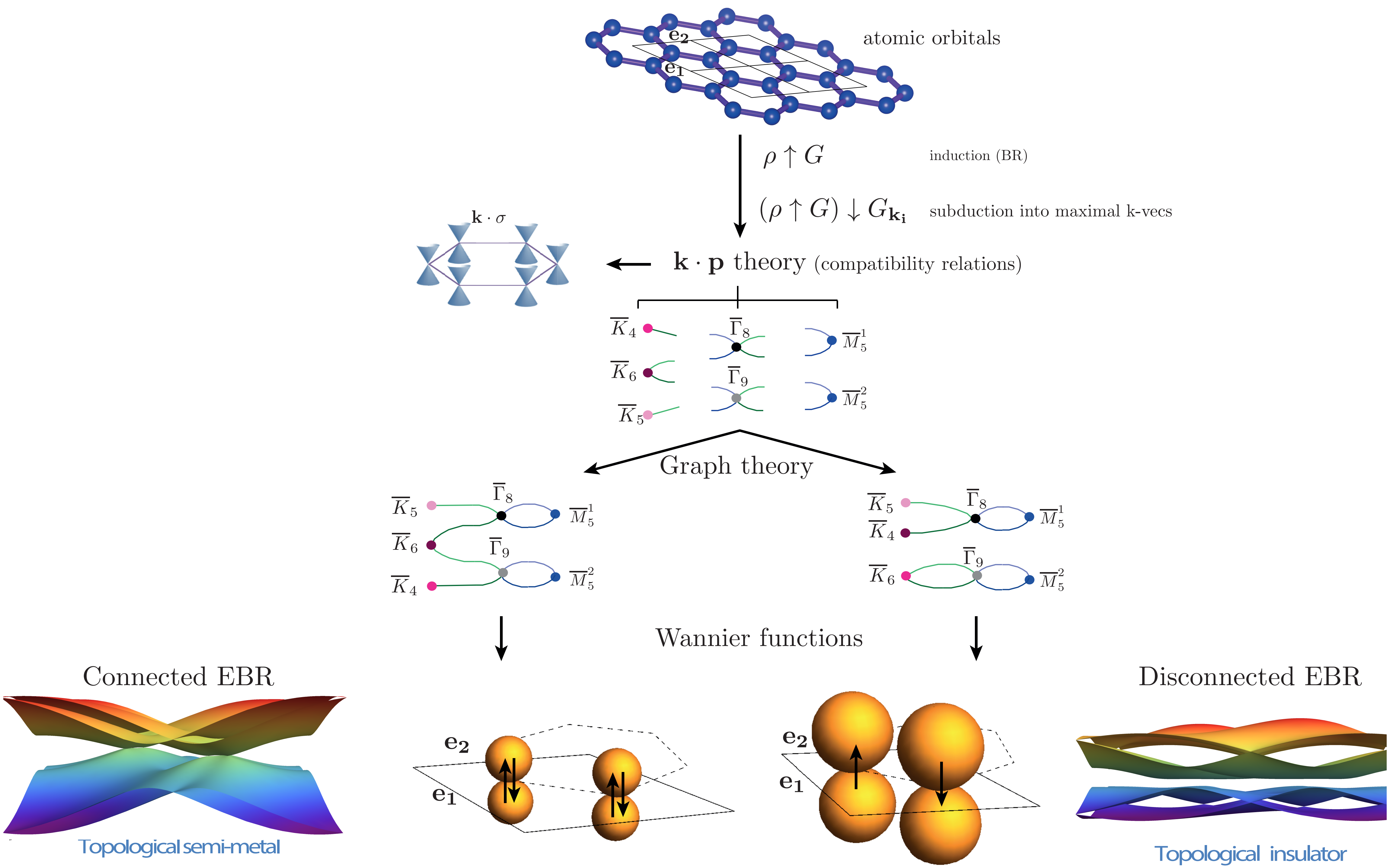


<u>Cannot</u> be described by localized Wannier functions while preserving symmetries (Soluyanov and Vanderbilt 2011)

Disconnected bands are topological because they lack localized Wannier functions that obey TR

Kane, Mele Phys. Rev. Lett (2005)

General method



Band Representations in the Bilbao Crystallographic Server

http://www.cryst.ehu.es/cryst/bandrep

Bilbao Crystallographic Server → BANDREP   Help

Band representations of the Double Space Groups

Band Representations

This program calculates the band representations (BR) induced from the irreps of the site-symmetry group of a given Wyckoff position.
Alternatively, it gives the set of elementary BRs of a Double Space Group.
In both cases, it can be chosen to get the BRs with or without time-reversal symmetry.
The program also indicates if the elementary BRs are decomposable or indecomposable. If it is decomposable, the program gives all the possible ways to decompose it.

Please, enter the sequential number of group as given in the *International Tables for Crystallography*, Vol. A   [choose it]

1. Get the elementary BRs without time-reversal symmetry [Elementary]
2. Get the elementary BRs with time-reversal symmetry [Elementary TR]
3. Get the BRs without time-reversal symmetry from a Wyckoff position [Wyckoff]
4. Get the BRs with time-reversal symmetry from a Wyckoff position [Wyckoff TR]

Bilbao Crystallographic Server
http://www.cryst.ehu.es

For comments, please mail to
administrador.bsc@ehu.eus

http://www.cryst.ehu.es/cryst/bandrep

Output

Elementary band-representations without time-reversal symmetry of the Double Space Group $I2_13$ (No. 199)

The first row shows the Wyckoff position from which the band representation is induced.
In parenthesis, the symbol of the point group isomorphic to the site-symmetry group.

The second row gives the symbol $\rho\uparrow G$, where ρ is the irrep of the site-symmetry group.
In parenthesis, the dimension of the representation.

The output shows the decomposition of the band representations into irreps of the little groups of the given k-vectors in the first column.
In parenthesis, the dimensions of the representations.

Minimal set of paths and compatibility relations to analyse the connectivity

Show all types of k-vectors

Wyckoff pos.	8a(3)	8a(3)	8a(3)	8a(3)	8a(3)	8a(3)	12b(2)	12b(2)	12b(2)	12b(2)
Band-Rep.	$A_1\uparrow G(4)$	$^1E\uparrow G(4)$	$^2E\uparrow G(4)$	$^1\overline{E}\uparrow G(4)$	$^2\overline{E}\uparrow G(4)$	$\overline{E}\uparrow G(4)$	$A\uparrow G(6)$	$B\uparrow G(6)$	$^1\overline{E}\uparrow G(6)$	$^2\overline{E}\uparrow G(6)$
Decomposable\ ndecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Decomposable
Γ:(0,0,0)	$\Gamma_1(1) \oplus \Gamma_4(3)$	$\Gamma_2(1) \oplus \Gamma_4(3)$	$\Gamma_3(1) \oplus \Gamma_4(3)$	$\overline{\Gamma}_5(2) \oplus \overline{\Gamma}_6(2)$	$\overline{\Gamma}_5(2) \oplus \overline{\Gamma}_7(2)$	$\overline{\Gamma}_6(2) \oplus \overline{\Gamma}_7(2)$	$\Gamma_1(1) \oplus \Gamma_2(1) \oplus \Gamma_3(1) \oplus \Gamma_4(3)$	$2\ \Gamma_4(3)$	$\overline{\Gamma}_5(2) \oplus \overline{\Gamma}_6(2) \oplus \overline{\Gamma}_7(2)$	$\overline{\Gamma}_5(2) \oplus \overline{\Gamma}_6(2) \oplus \overline{\Gamma}_7(2)$
H:(1,1,1)	$H_1(1) \oplus H_4(3)$	$H_2(1) \oplus H_4(3)$	$H_3(1) \oplus H_4(3)$	$\overline{H}_5(2) \oplus \overline{H}_6(2)$	$\overline{H}_5(2) \oplus \overline{H}_7(2)$	$\overline{H}_6(2) \oplus \overline{H}_7(2)$	$2\ H_4(3)$	$H_1(1) \oplus H_2(1) \oplus H_3(1) \oplus H_4(3)$	$\overline{H}_5(2) \oplus \overline{H}_6(2) \oplus \overline{H}_7(2)$	$\overline{H}_5(2) \oplus \overline{H}_6(2) \oplus \overline{H}_7(2)$
N:(1/2,1/2,0)	$2\ N_1(1) \oplus 2\ N_2(1)$	$2\ N_1(1) \oplus 2\ N_2(1)$	$2\ N_1(1) \oplus 2\ N_2(1)$	$2\ \overline{N}_3(1) \oplus 2\ \overline{N}_4(1)$	$2\ \overline{N}_3(1) \oplus 2\ \overline{N}_4(1)$	$2\ \overline{N}_3(1) \oplus 2\ \overline{N}_4(1)$	$3\ N_1(1) \oplus 3\ N_2(1)$	$3\ N_1(1) \oplus 3\ N_2(1)$	$4\ \overline{N}_3(1) \oplus 2\ \overline{N}_4(1)$	$2\ \overline{N}_3(1) \oplus 4\ \overline{N}_4(1)$
P:(1/2,1/2,1/2)	$P_1(2) \oplus P_3(2)$	$P_1(2) \oplus P_2(2)$	$P_2(2) \oplus P_3(2)$	$\overline{P}_6(1) \oplus \overline{P}_7(3)$	$\overline{P}_5(1) \oplus \overline{P}_7(3)$	$\overline{P}_4(1) \oplus \overline{P}_7(3)$	$P_1(2) \oplus P_2(2) \oplus P_3(2)$	$P_1(2) \oplus P_2(2) \oplus P_3(2)$	$2\ \overline{P}_7(3)$	$\overline{P}_4(1) \oplus \overline{P}_5(1) \oplus \overline{P}_6(1) \oplus \overline{P}_7(3)$

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Decomposable\ ndecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposab[illegible]e	Decomposable
Γ:(0,0,0)	$\Gamma_1(1) \oplus \Gamma_4(3)$	$\Gamma_2(1) \oplus \Gamma_4(3)$	$\Gamma_3(1) \oplus \Gamma_4(3)$	$\bar{\Gamma}_5(2) \oplus \bar{\Gamma}_6(2)$	$\bar{\Gamma}_5(2) \oplus \bar{\Gamma}_7(2)$	$\bar{\Gamma}_6(2) \oplus \bar{\Gamma}_7(2)$	$\Gamma_1(1) \oplus \Gamma_2(1) \oplus \Gamma_3(1) \oplus \Gamma_4(3)$	$2\,\Gamma_4(3)$	$\bar{\Gamma}_5(2) \oplus \bar{\Gamma}_6(2) \oplus \bar{\Gamma}$[illegible](2)	$\bar{\Gamma}_5(2) \oplus \bar{\Gamma}_6(2) \oplus \bar{\Gamma}_7(2)$
H:(1,1,1)	$H_1(1) \oplus H_4(3)$	$H_2(1) \oplus H_4(3)$	$H_3(1) \oplus H_4(3)$	$\bar{H}_5(2) \oplus \bar{H}_6(2)$	$\bar{H}_5(2) \oplus \bar{H}_7(2)$	$\bar{H}_6(2) \oplus \bar{H}_7(2)$	$2\,H_4(3)$	$H_1(1) \oplus H_2(1) \oplus H_3(1) \oplus H_4(3)$	$\bar{H}_5(2) \oplus \bar{H}_6(2) \oplus$ [illegible](2)	$\bar{H}_5(2) \oplus \bar{H}_6(2) \oplus \bar{H}_7(2)$
N:(1/2,1/2,0)	$2\,N_1(1) \oplus 2\,N_2(1)$	$2\,N_1(1) \oplus 2\,N_2(1)$	$2\,N_1(1) \oplus 2\,N_2(1)$	$2\,\bar{N}_3(1) \oplus 2\,\bar{N}_4(1)$	$2\,\bar{N}_3(1) \oplus 2\,\bar{N}_4(1)$	$2\,\bar{N}_3(1) \oplus 2\,\bar{N}_4(1)$	$3\,N_1(1) \oplus 3\,N_2(1)$	$3\,N_1(1) \oplus 3\,N_2(1)$	$4\,\bar{N}_3(1) \oplus 2\,\bar{N}_4$([illegible])	$2\,\bar{N}_3(1) \oplus 4\,\bar{N}_4(1)$
P:(1/2,1/2,1/2)	$P_1(2) \oplus P_3(2)$	$P_1(2) \oplus P_2(2)$	$P_2(2) \oplus P_3(2)$	$\bar{P}_6(1) \oplus \bar{P}_7(3)$	$\bar{P}_5(1) \oplus \bar{P}_7(3)$	$\bar{P}_4(1) \oplus \bar{P}_7(3)$	$P_1(2) \oplus P_2(2) \oplus P_3(2)$	$P_1(2) \oplus P_2(2) \oplus P_3(2)$	$2\,\bar{P}_7(3)$	$\bar{P}_4(1) \oplus \bar{P}_5(1) \oplus \bar{P}_6(1) \oplus \bar{P}_7(3)$

http://www.cryst.ehu.es/cryst/bandrep

Output

	branch 1	branch 2
1	$\bar{H}_5,\bar{\Gamma}_5,\bar{P}_5,\bar{P}_6,\bar{N}_4,\bar{N}_4$	$\bar{H}_6,\bar{H}_7,\bar{\Gamma}_6,\bar{\Gamma}_7,\bar{P}_4,\bar{P}_7,\bar{N}_3,\bar{N}_3,\bar{N}_4,\bar{N}_4$
2	$\bar{H}_6,\bar{\Gamma}_6,\bar{P}_4,\bar{P}_6,\bar{N}_4,\bar{N}_4$	$\bar{H}_7,\bar{H}_5,\bar{\Gamma}_5,\bar{\Gamma}_7,\bar{P}_5,\bar{P}_7,\bar{N}_3,\bar{N}_3,\bar{N}_4,\bar{N}_4$
3	$\bar{H}_7,\bar{\Gamma}_7,\bar{P}_4,\bar{P}_5,\bar{N}_4,\bar{N}_4$	$\bar{H}_5,\bar{H}_6,\bar{\Gamma}_5,\bar{\Gamma}_6,\bar{P}_6,\bar{P}_7,\bar{N}_3,\bar{N}_3,\bar{N}_4,\bar{N}_4$

Wyckoff pos.	8	…	(2)
Band-Rep.	A_1	…	G(6)
Decomposable\ Indecomposable	Indeco	…	osable
Γ:(0,0,0)	$\Gamma_1(1)$	…	$(2) \oplus \bar{\Gamma}_7(2)$
H:(1,1,1)	$H_1(1)$	…	$(2) \oplus \bar{H}_7(2)$
N:(1/2,1/2,0)	$2\ N_1(1)$	…	$4\ \bar{N}_4(1)$
P:(1/2,1/2,1/2)	$P_1(2)$	…	$\bar{P}_6(1) \oplus \bar{P}_7(3)$

http://www.cryst.ehu.es/cryst/bandrep

Output

Elementary band-representations without time-reversal symmetry of the Double Space Group $I2_13$ (No. 199)

The first row shows the Wyckoff position from which the band representation is induced.
In parenthesis, the symbol of the point group isomorphic to the site-symmetry group.

The second row gives the symbol ρ↑G, where ρ is the irrep of the site-symmetry group.
In parenthesis, the dimension of the representation.

The output shows the decomposition of the band representations into irreps of the little groups of the given k-vectors in the first column.
In parenthesis, the dimensions of the representations.

Minimal set of paths and compatibility relations to analyse the connectivity

Show all types of k-vectors

Wyckoff pos.	8a(3)	8a(3)	8a(3)	8a(3)	8a(3)	8a(3)	12b(2)	12b(2)	12b(2)	12b(2)
Band-Rep.	$A_1\uparrow G(4)$	$^1E\uparrow G(4)$	$^2E\uparrow G(4)$	$^1\bar{E}\uparrow G(4)$	$^2\bar{E}\uparrow G(4)$	$\bar{E}\uparrow G(4)$	$A\uparrow G(6)$	$B\uparrow G(6)$	$^1\bar{E}\uparrow G(6)$	$^2\bar{E}\uparrow G(6)$
Decomposable\ Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Decomposable
Γ:(0,0,0)	$\Gamma_1(1) \oplus \Gamma_4(3)$	$\Gamma_2(1) \oplus \Gamma_4(3)$	$\Gamma_3(1) \oplus \Gamma_4(3)$	$\bar{\Gamma}_5(2) \oplus \bar{\Gamma}_6(2)$	$\bar{\Gamma}_5(2) \oplus \bar{\Gamma}_7(2)$	$\bar{\Gamma}_6(2) \oplus \bar{\Gamma}_7(2)$	$\Gamma_1(1) \oplus \Gamma_2(1) \oplus \Gamma_3(1) \oplus \Gamma_4(3)$	$2\,\Gamma_4(3)$	$\bar{\Gamma}_5(2) \oplus \bar{\Gamma}_6(2) \oplus \bar{\Gamma}_7(2)$	$\bar{\Gamma}_5(2) \oplus \bar{\Gamma}_6(2) \oplus \bar{\Gamma}_7(2)$
H:(1,1,1)	$H_1(1) \oplus H_4(3)$	$H_2(1) \oplus H_4(3)$	$H_3(1) \oplus H_4(3)$	$\bar{H}_5(2) \oplus \bar{H}_6(2)$	$\bar{H}_5(2) \oplus \bar{H}_7(2)$	$\bar{H}_6(2) \oplus \bar{H}_7(2)$	$2\,H_4(3)$	$H_1(1) \oplus H_2(1) \oplus H_3(1) \oplus H_4(3)$	$\bar{H}_5(2) \oplus \bar{H}_6(2) \oplus \bar{H}_7(2)$	$\bar{H}_5(2) \oplus \bar{H}_6(2) \oplus \bar{H}_7(2)$
N:(1/2,1/2,0)	$2\,N_1(1) \oplus 2\,N_2(1)$	$2\,N_1(1) \oplus 2\,N_2(1)$	$2\,N_1(1) \oplus 2\,N_2(1)$	$2\,\bar{N}_3(1) \oplus 2\,\bar{N}_4(1)$	$2\,\bar{N}_3(1) \oplus 2\,\bar{N}_4(1)$	$2\,\bar{N}_3(1) \oplus 2\,\bar{N}_4(1)$	$3\,N_1(1) \oplus 3\,N_2(1)$	$3\,N_1(1) \oplus 3\,N_2(1)$	$4\,\bar{N}_3(1) \oplus 2\,\bar{N}_4(1)$	$2\,\bar{N}_3(1) \oplus 4\,\bar{N}_4(1)$
P:(1/2,1/2,1/2)	$P_1(2) \oplus P_3(2)$	$P_1(2) \oplus P_2(2)$	$P_2(2) \oplus P_3(2)$	$\bar{P}_6(1) \oplus \bar{P}_7(3)$	$\bar{P}_5(1) \oplus \bar{P}_7(3)$	$\bar{P}_4(1) \oplus \bar{P}_7(3)$	$P_1(2) \oplus P_2(2) \oplus P_3(2)$	$P_1(2) \oplus P_2(2) \oplus P_3(2)$	$2\,\bar{P}_7(3)$	$\bar{P}_4(1) \oplus \bar{P}_5(1) \oplus \bar{P}_6(1) \oplus \bar{P}_7(3)$

http://www.cryst.ehu.es/cryst/bandrep

Output

Maximal k-vec	Compatibility relations	Intermediate path	Compatibility relations	Maximal k-vec
Γ:(0,0,0)	$\Gamma_1(1)\rightarrow\Delta_1(1)$ $\Gamma_2(1)\rightarrow\Delta_1(1)$ $\Gamma_3(1)\rightarrow\Delta_1(1)$ $\Gamma_4(3)\rightarrow\Delta_1(1)\oplus 2\ \Delta_2(1)$ $\overline{\Gamma}_5(2)\rightarrow\overline{\Delta}_3(1)\oplus\overline{\Delta}_4(1)$ $\overline{\Gamma}_6(2)\rightarrow\overline{\Delta}_3(1)\oplus\overline{\Delta}_4(1)$ $\overline{\Gamma}_7(2)\rightarrow\overline{\Delta}_3(1)\oplus\overline{\Delta}_4(1)$	Δ:(0,v,0)	$H_1(1)\rightarrow\Delta_2(1)$ $H_2(1)\rightarrow\Delta_2(1)$ $H_3(1)\rightarrow\Delta_2(1)$ $H_4(3)\rightarrow 2\ \Delta_1(1)\oplus\Delta_2(1)$ $\overline{H}_5(2)\rightarrow\overline{\Delta}_3(1)\oplus\overline{\Delta}_4(1)$ $\overline{H}_6(2)\rightarrow\overline{\Delta}_3(1)\oplus\overline{\Delta}_4(1)$ $\overline{H}_7(2)\rightarrow\overline{\Delta}_3(1)\oplus\overline{\Delta}_4(1)$	H:(1,1,1)
Γ:(0,0,0)	$\Gamma_1(1)\rightarrow\Lambda_1(1)$ $\Gamma_2(1)\rightarrow\Lambda_2(1)$ $\Gamma_3(1)\rightarrow\Lambda_3(1)$ $\Gamma_4(3)\rightarrow\Lambda_1(1)\oplus\Lambda_2(1)\oplus\Lambda_3(1)$ $\overline{\Gamma}_5(2)\rightarrow\overline{\Lambda}_5(1)\oplus\overline{\Lambda}_6(1)$ $\overline{\Gamma}_6(2)\rightarrow\overline{\Lambda}_4(1)\oplus\overline{\Lambda}_6(1)$ $\overline{\Gamma}_7(2)\rightarrow\overline{\Lambda}_4(1)\oplus\overline{\Lambda}_5(1)$	Λ:(-u,u,-u)	$H_1(1)\rightarrow\Lambda_1(1)$ $H_2(1)\rightarrow\Lambda_2(1)$ $H_3(1)\rightarrow\Lambda_3(1)$ $H_4(3)\rightarrow\Lambda_1(1)\oplus\Lambda_2(1)\oplus\Lambda_3(1)$ $\overline{H}_5(2)\rightarrow\overline{\Lambda}_5(1)\oplus\overline{\Lambda}_6(1)$ $\overline{H}_6(2)\rightarrow\overline{\Lambda}_4(1)\oplus\overline{\Lambda}_6(1)$ $\overline{H}_7(2)\rightarrow\overline{\Lambda}_4(1)\oplus\overline{\Lambda}_5(1)$	H:(1,1,1)
Γ:(0,0,0)	$\Gamma_1(1)\rightarrow\Lambda_1(1)$ $\Gamma_2(1)\rightarrow\Lambda_2(1)$ $\Gamma_3(1)\rightarrow\Lambda_3(1)$ $\Gamma_4(3)\rightarrow\Lambda_1(1)\oplus\Lambda_2(1)\oplus\Lambda_3(1)$ $\overline{\Gamma}_5(2)\rightarrow\overline{\Lambda}_5(1)\oplus\overline{\Lambda}_6(1)$ $\overline{\Gamma}_6(2)\rightarrow\overline{\Lambda}_4(1)\oplus\overline{\Lambda}_6(1)$ $\overline{\Gamma}_7(2)\rightarrow\overline{\Lambda}_4(1)\oplus\overline{\Lambda}_5(1)$	Λ:(-u,u,-u)	$P_1(2)\rightarrow\Lambda_1(1)\oplus\Lambda_2(1)$ $P_2(2)\rightarrow\Lambda_2(1)\oplus\Lambda_3(1)$ $P_3(2)\rightarrow\Lambda_1(1)\oplus\Lambda_3(1)$ $\overline{P}_4(1)\rightarrow\overline{\Lambda}_4(1)$ $\overline{P}_5(1)\rightarrow\overline{\Lambda}_5(1)$ $\overline{P}_6(1)\rightarrow\overline{\Lambda}_6(1)$ $\overline{P}_7(3)\rightarrow\overline{\Lambda}_4(1)\oplus\overline{\Lambda}_5(1)\oplus\overline{\Lambda}_6(1)$	P:(1/2,1/2,1/2)

Wyckoff pos.		
Band-Rep.	A	
Decomposable\ Indecomposable	Indec	
Γ:(0,0,0)	Γ_1(	)
H:(1,1,1)	H_1(	)
N:(1/2,1/2,0)	2 N_1(	
P:(1/2,1/2,1/2)	P_1(	$\overline{P}_7(3)$

Materials?

We tabulated all the different EBRs (10403) of all the 230 SG.

SG	MWP	WM	PG	Irrep	Dim	KR	Bands	Re	E	PE	SG	MWP	WM	PG	Irrep	Dim	KR	Bands	Re	E	PE
1	$1a$	1	1	Γ_1	1	1	1	1	e	e	131	$2d$	2	8	Γ_2^-	1	1	2	1	e	e
1	$1a$	1	1	$\bar{\Gamma}_2$	1	2	2	2	e	e	131	$2d$	2	8	Γ_4^+	1	1	2	1	e	e
2	$1a$	1	2	Γ_1^+	1	1	1	1	e	e	131	$2d$	2	8	Γ_4^-	1	1	2	1	e	e
2	$1a$	1	2	Γ_1^-	1	1	1	1	e	e	131	$2d$	2	8	Γ_3^+	1	1	2	1	e	e
2	$1a$	1	2	$\bar{\Gamma}_3$	1	2	2	2	e	e	131	$2d$	2	8	Γ_3^-	1	1	2	1	e	e
2	$1a$	1	2	$\bar{\Gamma}_2$	1	2	2	2	e	e	131	$2d$	2	8	$\bar{\Gamma}_5$	2	1	4	1	e	e
2	$1b$	1	2	Γ_1^+	1	1	1	1	e	e	131	$2d$	2	8	$\bar{\Gamma}_6$	2	1	4	1	e	e
2	$1b$	1	2	Γ_1^-	1	1	1	1	e	e	131	$2e$	2	14	Γ_1	1	1	2	1	e	e
2	$1b$	1	2	$\bar{\Gamma}_3$	1	2	2	2	e	e	131	$2e$	2	14	Γ_4	1	1	2	1	e	e

SG: Space Group
MWP: Maximal Wyckoff Position
WM: Wyckoff multiplicity in the primitive cell
PG: Point group number of the site-symmetry
Irrep: Name of the Irrep of the site-symmetry for each BR

KR: 1 for PEBR, 2 for EBR (f and s)
Bands: Total number of bands
Re: 1 for TRS at each k, 2 for connection with its conjugate
E: e for elementary, c for composite
PE: e for elementary, c for composite

Materials?

We tabulated all the different EBRs (10403) of all the 230 SG.

SG	MWP	WM	PG	Irrep	Dim	KR	Bands	Re	E	PE	SG	MWP	WM	PG	Irrep	Dim	KR	Bands	Re	E	PE
1	$1a$	1	1	Γ_1	1	1	1	1	e	e	131	$2d$	2	8	Γ_2^-	1	1	2	1	e	e
1	$1a$	1	1	$\bar{\Gamma}_2$	1	2	2	2	e	e	131	$2d$	2	8	Γ_4^+	1	1	2	1	e	e
2	$1a$	1	2	Γ_1^+	1	1	1	1	e	e	131	$2d$	2	8	Γ_4^-	1	1	2	1	e	e
2	$1a$	1	2	Γ_1^-	1	1	1	1	e	e	131	$2d$	2	8	Γ_3^+	1	1	2	1	e	e
2	$1a$	1	2	$\bar{\Gamma}_3$	1	2	2	2	e	e	131	$2d$	2	8	Γ_3^-	1	1	2	1	e	e
2	$1a$	1	2	$\bar{\Gamma}_2$	1	2	2	2	e	e	131	$2d$	2	8	$\bar{\Gamma}_5$	2	1	4	1	e	e
2	$1b$	1	2	Γ_1^+	1	1	1	1	e	e	131	$2d$	2	8	$\bar{\Gamma}_6$	2	1	4	1	e	e
2	$1b$	1	2	Γ_1^-	1	1	1	1	e	e	131	$2e$	2	14	Γ_1	1	1	2	1	e	e
2	$1b$	1	2	$\bar{\Gamma}_3$	1	2	2	2	e	e	131	$2e$	2	14	Γ_4	1	1	2	1	e	e

Classification: 2 indices (m,n)

- Type(1,1): Fermi at single EBR ➔ Gap ➔ TI
- Type(1,2): EBR at Fermi ➔ Gap ➔ 2 PEBRs ➔ TIs
- Type(2,2): More than one EBR at Fermi ➔ Gap closes and reopens ➔ 2 PEBRs
- Semimetals: electron number is a fraction of the EBR connectivity

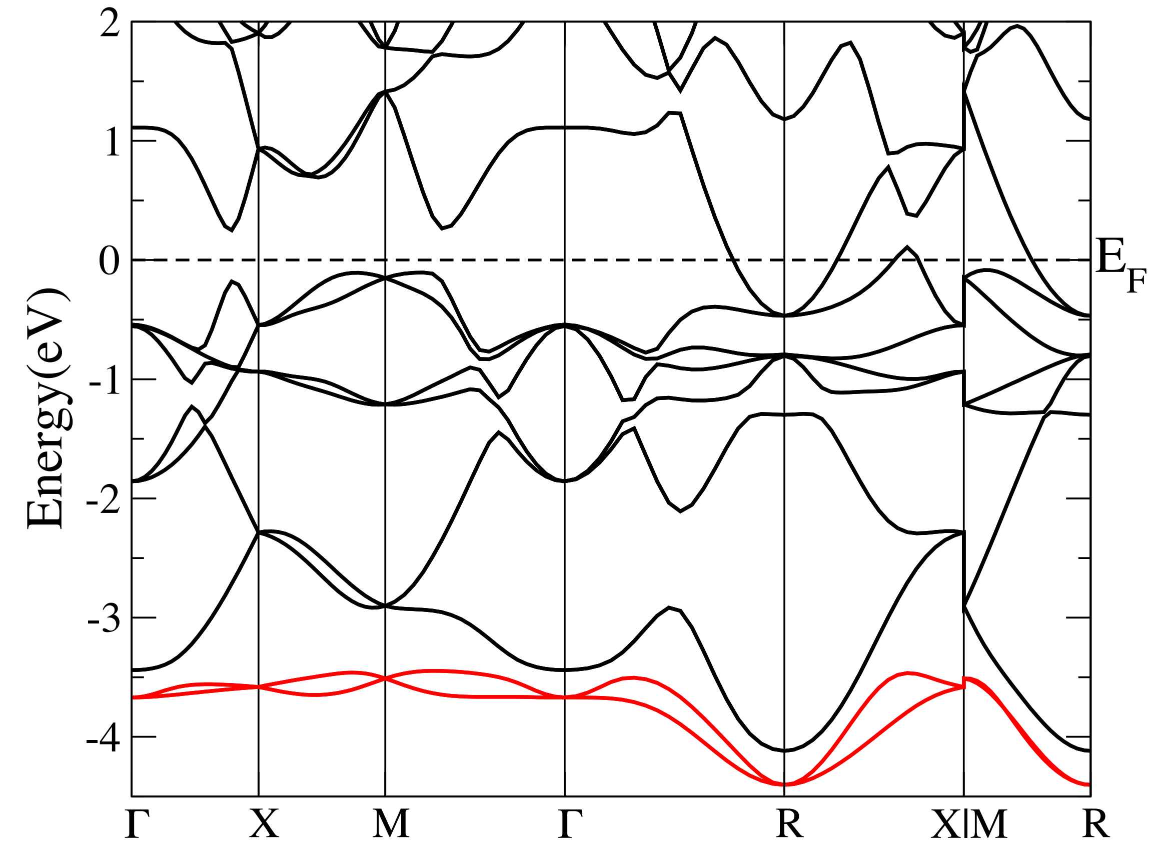
Type(1,1):

Disconnected EBRs

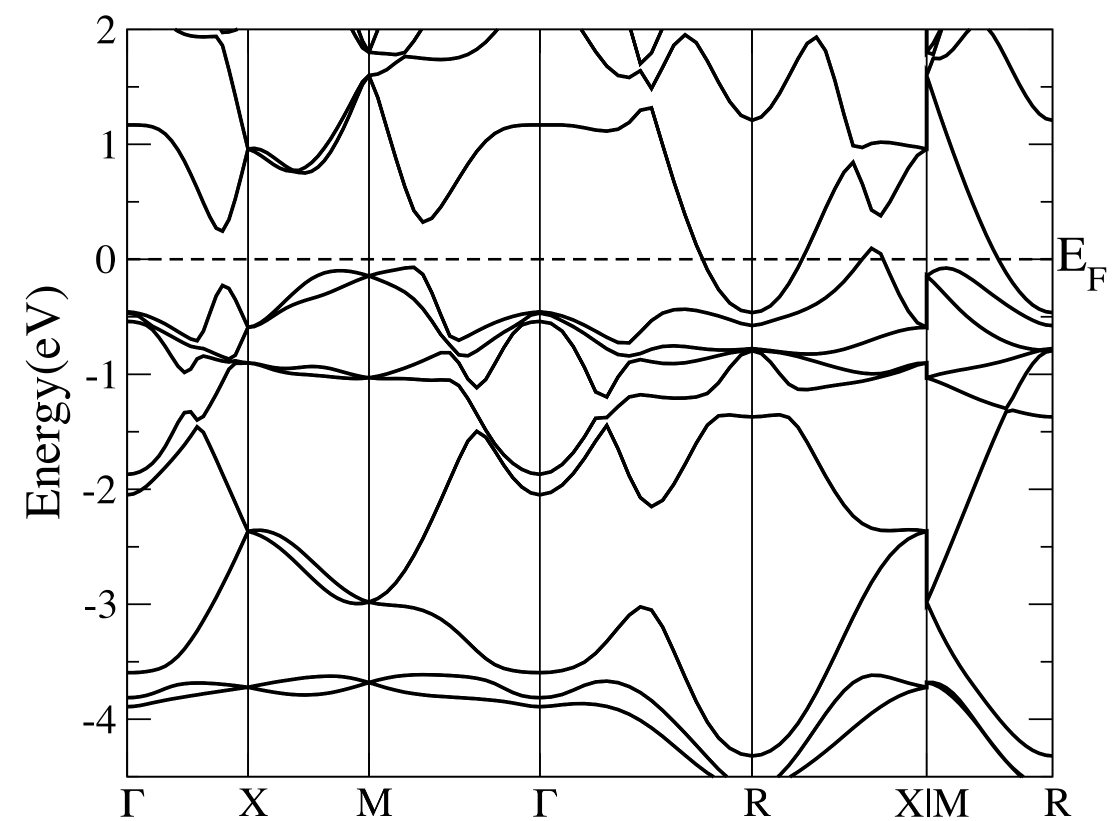
SG	WP	Irrep
224	2a	-GM8
224	4b	-GM5-GM4
224	4b	-GM7-GM6
224	4b	-GM8
224	4b	-GM9
224	4c	-GM5-GM4
224	4c	-GM7-GM6
224	4c	-GM8
224	4c	-GM9
224	6d	GM5
224	6d	-GM6
224	6d	-GM7
224	12f	-GM5

→ Pb in 4c

Pb_2O in $Pn\bar{3}m$ (224)



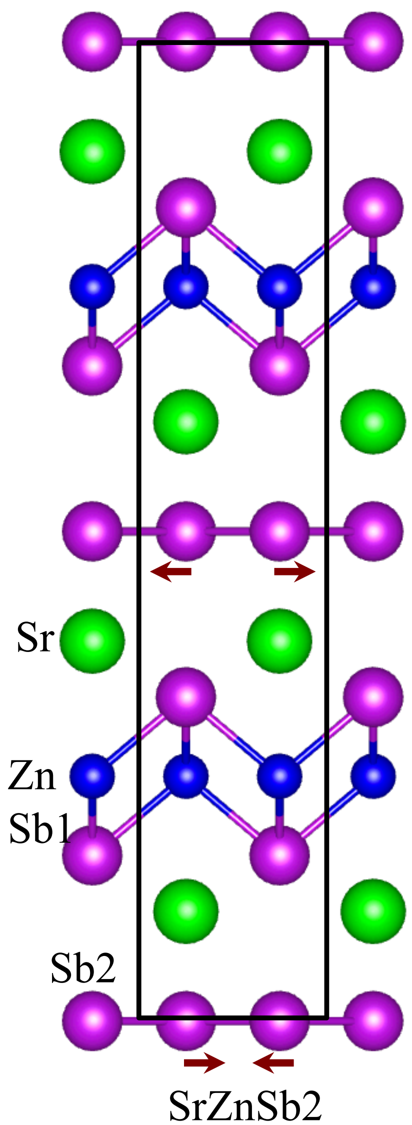
$P4_2/nnm$ (134) gap is opened under uniaxial strain



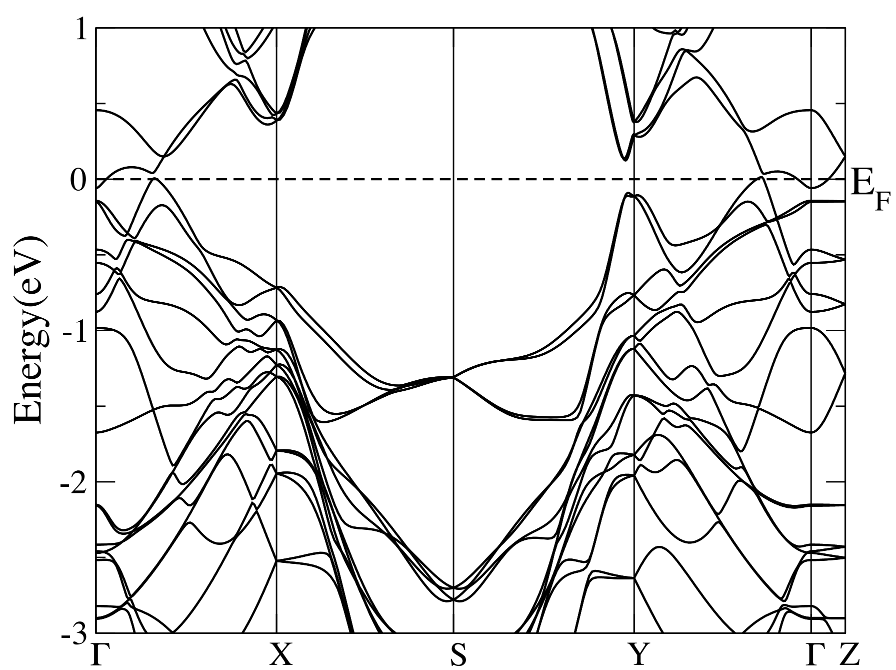
Type(1,2):

1 EBR without SOC
2 pEBR with SOC

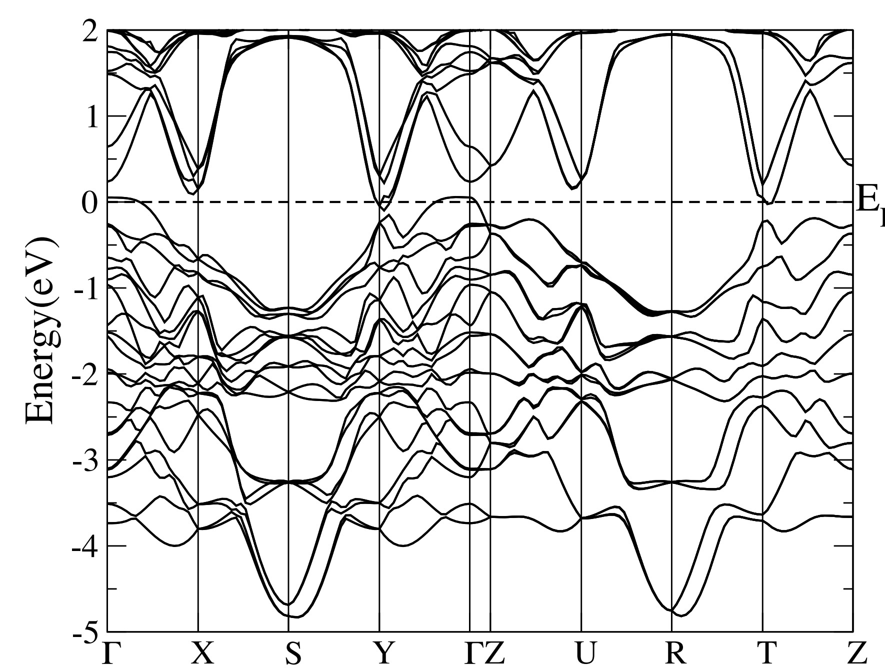
Pnma (62)



- Without SOC these materials are filling enforced semimetals
- It splits into a topologically disconnected band representations when SOC is turned on



(a)



(b)

We found 58 new candidates: $SrZnSb_2$ (a), LaSbTe (b), AAgX2 (A: rare earth metal, X: P, As, Sb Bi)

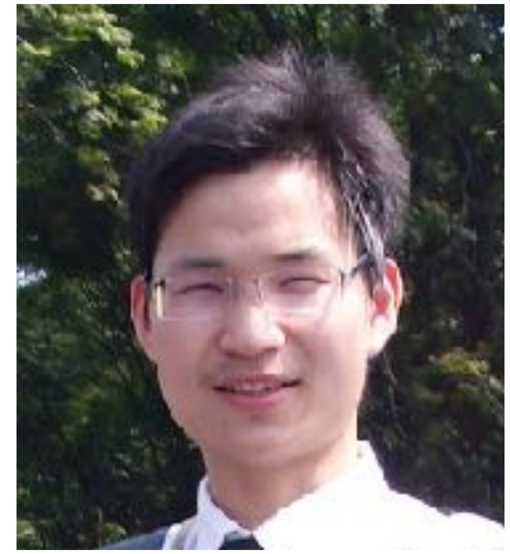
Outlook

- Predictive theory of topological bands that makes the link between real space orbitals and momentum space topology
- Gives a prescription on how to built topological bands from orbitals
- Finds a large amount of materials
- Magnetic symmetry groups are next

Collaborators

Barry Bradley
(Princeton)

Jennifer Cano
(Princeton)



Zhijun Wang
(Princeton)

Luis Elcoro (EHU)

Claudia Felser
(Max Planck Institute
Chem. Phys of Solids)

Mois Aroyo (EHU)

Andrei Bernevig
(Princeton)